

Valorisation of liquorice (*Glycyrrhiza*) roots: antimicrobial activity and cytotoxicity of prenylated (iso)flavonoids and chalcones from liquorice spent (*G. glabra*, *G. inflata*, and *G. uralensis*)

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A. Phenolics subclasses

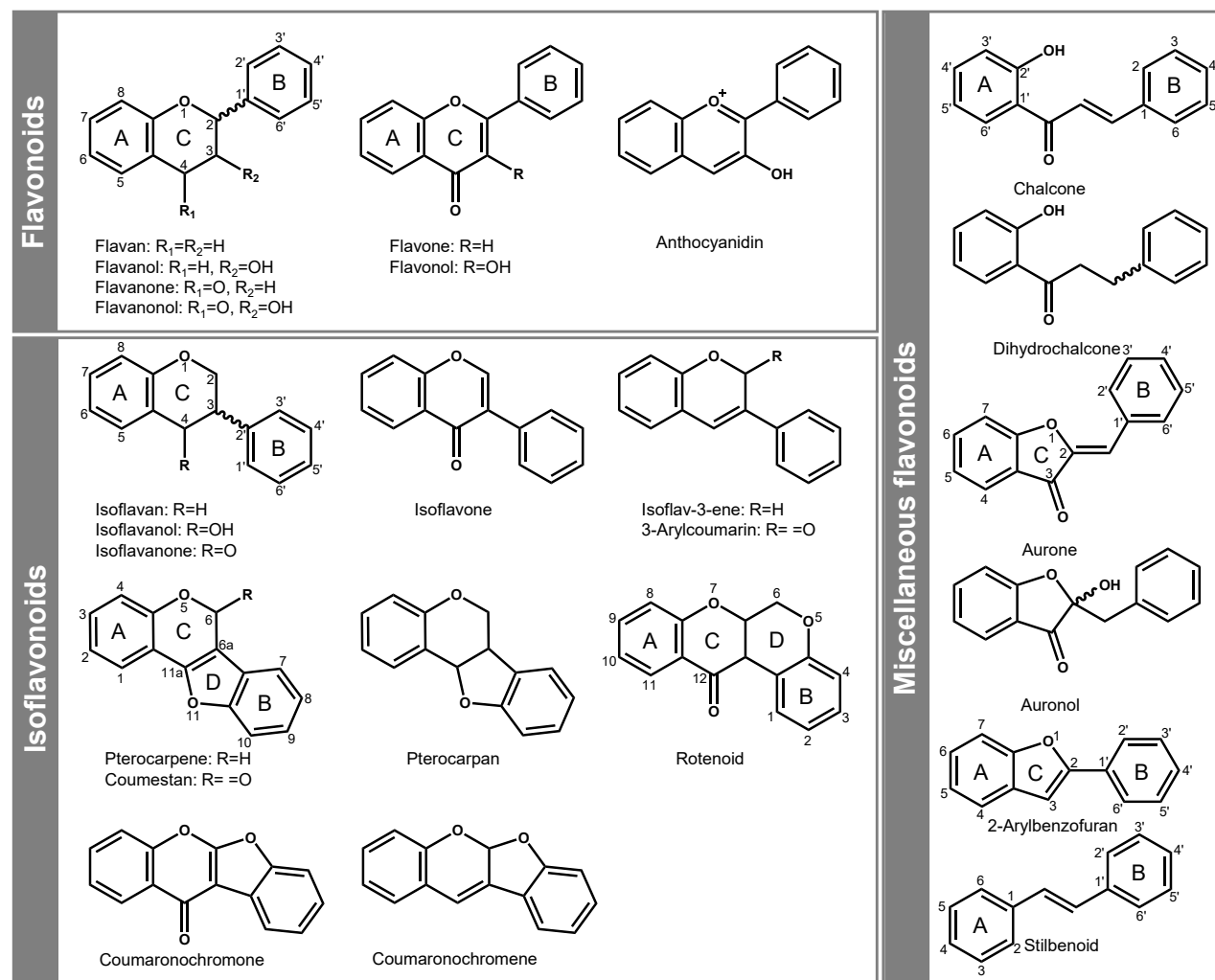


Figure A1. Flavonoid, isoflavonoid, and miscellaneous flavonoid subclasses (together called phenolics). IUPAC numbering of the different subclasses is shown (skeletons without numbering are numbered similarly as the first skeleton of their class).

B. Diagnostic UV_{max}, neutral losses, and *retro*-Diels Alder fragmentation for (iso)flavonoid and chalcone identification

Table B1. Summary of diagnostic UV_{max} (nm) and *retro*-Diels Alder (RDA) fragmentations for different (iso)flavonoid subclasses and chalcones in positive ionisation mode. Typical UV_{max} is based on work by Mabry and co-workers¹, and typical RDA fragmentation is based on research by van Dinteren *et al.*² and Araya-Cloutier *et al.*³

(Iso)flavonoid subclass	UV _{max} (±5 nm)	Diagnostic RDA fragmentation
<u>Flavonoids</u>		
Flavone	270, 325-340	^{1,3} A/B ⁺ , ^{0,2} B ⁺ , ^{0,4} B ⁺
Flavanone	280-290	^{1,2} A/B ⁺ , ^{1,3} A/B ⁺
Flavonol	250-280, 300-350	^{0,2} A ⁺ , ^{1,3} A ⁺ , ^{1,4} A ⁺ +2H, ^{1,3} B ⁺ -2H
Flavanonol	275-280, 310-315	^{1,4} B ⁺ , ^{0,2} B ⁺
<u>Isoflavonoids</u>		
Isoflavone	250-260	^{1,3} A/B ⁺ , -B-ring, B-ring
Isoflavanone	270-295	^{1,3} A/B ⁺ , ^{0,4} B ⁺ , ^{2,3} B ⁺
Isoflavan	270-285	^{1,3} A/B ⁺
Pterocarpan	280-310	^{1,4} A/B ⁺ , ^{2,4} A/B ⁺
Pterocarpene	280-310, 330-365	-
Coumestan	340-350	-
3-Arylcoumarin	340-350	^{2,4} A/B ⁺
<u>Miscellaneous</u>		
Chalcone	220-270, 300-320, 340-390	⁰ A/B ⁺ , ¹ A/B ⁺

C. Molar extinction coefficient of (iso)flavonoids and chalcones

Table C1. Molar extinction coefficients (ϵ) of (iso)flavonoids and chalcones used for quantification of compounds in EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent.

Compound	Subclass	ϵ (AU/M·cm) at 280 nm	Reference
Glabridin	Isoflavan	11175	4
Glabrene	Isoflav-3-ene	9708	4
Glabrol	Flavanone	11748	4
Hispaglabridin A	Isoflavan	9145	4
Hispaglabridin B	Isoflavan	12254	4
Naringenin (3 -OH groups)	Flavanone	12592	
8-Prenylnaringenin (3 -OH groups)	Flavanone	15530	5
Eriodictyol (4 -OH groups)	Flavanone	14221	6
Apigenin	Flavone	14253	6
Kaempferol	Flavonol	11888	6
Dalbergioidin	Isoflavanone	19432	7
Daidzein (2 -OH groups)	Isoflavone	13782	6
Genistein (3 -OH groups)	Isoflavone	11961	6
3'-OH-Genistein (4 -OH groups)	Isoflavone	12938	8
Glyceollin I	Pterocarpan	8634	9
Coumestrol	Coumestan	5412	10
Licochalcone A	Chalcone	5208	11
Glycy coumarin	3-Arylcoumarin	8997	12

D. Optimal growth parameters of the various microorganisms

Table D1. Optimal growth parameters of the various microorganisms used in this study.

Bacteria/ Yeast	Culture medium	Incubation temp. (°C)	Incubation time (h)	Initial inoculum (Log ₁₀ CFU mL ⁻¹)
<i>L. buchneri</i>				
ATCC 4005	MRS/YPD ^a	37	72	5.74±0.29
L4	MRS/YPD ^a	37	72	5.13±0.05
<i>S. mutans</i>				
ATCC 27175	TSA/TSB	37	24	4.85±0.13
<i>S. aureus</i>				
ATCC 25923	TSA/TSB	37	24	4.88±0.34
<i>E. coli</i>				
K12	TSA/TSB	37	24	5.01±0.36
O54:H21	TSA/TSB	37	24	5.20±0.05
O88:H8	TSA/TSB	37	24	5.14±0.05
<i>Y. lipolytica</i>				
Food isolate	YPD	25	25	4.90±0.17
<i>Z. parabailli</i>				
ATCC 60483	YPD	30	48	5.09±0.22
UL 3699	YPD	30	48	5.24±0.15

^aYPD broth was only used during the broth microdilution assay, due to solubility problems of the liquorice extracts in MRS. To confirm cell counts, MRS agar was used.

E. Tentative identification of prenylated phenolics in EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent by IT-MSⁿ

Table E1. Tentative identification of prenylated phenolics in EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent (**Figure 2**) and the spectrometric data obtained using negative- and positive ionisation mode ESI-IT-MSⁿ. Numbers refer to peaks in **Figure 2**. Bold number indicate the same compound between *Glycyrrhiza* species (G = *G. glabra*, I = *G. inflata*, and U = *G. uralensis*).

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
<i>G. glabra</i>											
G-I-U-1	3.82	<u>278</u> , 314	C ₁₅ H ₁₂ O ₄	Flavanone	255	135 (100)	257	137 (91), 147 (90), 13 (15), 211 (37), 239 (100), 242 (37)	211 (100)	0	Liquiritigenin
G-I-U-2	9.07	370	C ₁₅ H ₁₂ O ₄	Chalcone	255	135 (100)	257	137 (91), 147 (94), 163 (16), 211 (36), 239 (100), 242 (40)	211 (100)	0	Isoliquiritigenin
G-I-U-3	9.99	262 ^{sh} , 306	C ₁₆ H ₁₂ O ₄	Isoflavone	267	252 (100)	269	107 (16), 213 (35), 237 (43), 241 (11), 254 (100), 269 (81)	118 (15), 136 (17), 226 (12), 237 (100), 253 (21)	0	Formononetin
G4	15.42	338	C ₂₀ H ₁₈ O ₄	Flavone	321	266 (100), 321 (16)	323	267 (100)	121 (11), 149 (100), 239 (19)	1, 3,3-DMA, C8 A-ring	7,4'-Dihydroxy-8-prenylflavone
G-I-5	18.67	298, <u>326</u>	C ₂₀ H ₁₈ O ₄	Isoflav-3-ene	321	175 (12), 265 (37), 266 (16), 277 (100), 278 (30), 291 (12), 293 (12), 303 (30), 305 (51), 306 (78), 321 (10)	322 ^(c)	123 (10), 147 (37), 163 (20), 189 (68), 213 (37), 266 (10), 267 (10), 279 (100), 280 (50), 281 (12), 295 (39), 305 (14), 307 (31), 308 (17), 322 (12)	223 (9), 279 (100), 280 (30)	1, 2,2-DMP, C3' B-ring	Glabrene
G6	19.00	278	C ₂₀ H ₂₀ O ₄	Isoflavan	341 ^(d)	283 (100), 323 (5)	325	123 (32), 189(100), 203 (25), 215 (13)	147(100), 171 (25)	1, 2,2-DMP, C3' B-ring	Phaseollinisoflavan
G7	21.14	278, <u>322</u>	C ₁₉ H ₁₆ O ₄	n.i.	307	247 (13), 261 (47), 262 (13), 263 (87), 264 (26), 265 (12), 277 (22), 278 (17), 279 (16), 288 (55), 289 (90), 291 (93), 292 (100), 305 (24), 306 (31), 307 (38)	308 ^(e)	281 (46), 293(100), 294 (30)	265 (85), 266 (23), 293(100), 294 (18)	0	n.i. Not prenylated
G8	21.14	278, <u>322</u>	C ₂₀ H ₁₆ O ₅	Isoflavone	335	161 (24), 291 (76), 292 (35), 305 (13), 307 (100), 317 (27),	337	283 (14), 295 (100), 309 (26), 319 (13)	133 (15), 239 (97), 267 (100)	1, 2,2-DMP, C3' B-ring	Glabrone

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
						320 (53), 335 (23)					
G-I-9	23.00	350	C ₂₀ H ₁₆ O ₅	3-Arylcoumarin	335	213 (15), 291 (100), 292 (13), 320 (19)	337	267 (11), 283 (34), 295 (100), 296 (10), 309 (41), 319 (41)	137 (12), 239 (78), 267 (100), 268 (10), 277 (8), 295 (87)	1, 2,2-DMP, C3' B-ring	Glabrocoumarin
G10	23.22	366	C ₂₁ H ₂₂ O ₅	Chalcone	353	177 (100)	355	137 (26), 177 (16), 231 (48), 271 (24), 281 (11), 299 (100), 327 (29), 337 (47)	137 (100), 281 (30)	1, 3,3-DMA, C3' B-ring	Licoagrochalcone C
G-I-11	24.59	<u>278</u> , 322	C ₂₀ H ₂₀ O ₄	Isoflavan	323	135 (100), 175 (29), 187 (16), 201 (83), 213 (44), 253 (14), 264 (11), 279 (27), 305 (27), 308 (18)	325	189 (100), 203 (18)	147 (100), 171 (24)	1, 2,2-DMP, C8 A-ring	Glabridin
G12	25.56	<u>286</u> , 318	C ₂₅ H ₂₈ O ₅	Flavanonol	407	363 (11), 379 (100), 380 (10)	409	203 (63), 205 (37), 247 (32), 335 (14), 353 (23), 363 (39), 391 (100)	294 (14), 307 (19), 335 (23), 363 (100)	2, 3,3-DMA, C8 A-ring and C3' B-ring	3-Hydroxyglabrol
G13	25.77	282, <u>338</u>	C ₂₀ H ₁₈ O ₄	Pterocarpan	321	n.d.	323	123 (100), 147 (45), 163 (16), 189 (64), 213 (25), 267 (3), 281 (4), 295 (21), 307 (35), 308 (26)	95 (100)	1, 2,2-DMP, C3' B-ring	Phaseollin
G14	25.77	282, <u>338</u>	C ₂₁ H ₂₀ O ₅	n.i.	351	336 (100)	353	269 (17), 285 (8), 297 (100), 325 (47)	227 (23), 241 (90), 255 (12), 269 (100)	1, 3,3-DMA, C3' B-ring	n.i. B-ring 3,3-DMA prenylated
G15	26.96	342	C ₂₅ H ₂₄ O ₅	n.i.	423 ^(d)	203 (17), 219 (30), 235 (50), 351 (30), 379 (13), 395 (27), 405 (100)	406 ^(c)	363 (100), 387 (36), 388 (13)	345 (100)	1, 2,2-DMP, n.i.	n.i. 2,2-DMP prenylated
G16	27.36	282, <u>330</u>	C ₂₅ H ₂₄ O ₅	Isoflavone	403	157 (26), 201 (84), 334 (46), 347 (30), 348 (34), 359 (30), 360 (16), 375 (100), 385 (47), 388 (16), 403 (37)	405	203 (100), 337 (21), 349 (5), 377 (12)	247 (22), 149 (13), 161 (100), 163 (11), 175 (29), 185 (73)	2, 2,2-DMP on C8 A- ring and 3,3-DMA on C3' B-ring	Scanderone
G17	27.36	282, <u>330</u>	C ₂₅ H ₂₄ O ₄	Flavone	387	n.d.	389	333 (100), 334 (31), 389 (27), 390 (10)	235 (14), 249 (10), 259 (10), 263 (32), 277 (36), 279 (46), 287 (12), 290 (20), 291 (50), 304 (12), 305 (100), 306 (20), 315 (25), 318 (63), 319 (32), 333 (17)	2, 3,3-DMA on C6 A- ring and 2,2-DMP on C3' B-ring	Kanzonol E
G18	28.23	282, 338	C ₂₅ H ₃₀ O ₅	2'-hydroxy- dihydrochalcone	409	217 (14), 235 (100), 391 (27)	411	175 (34), 337 (16), 355 (19), 365 (9), 393 (100)	175(100), 337 (33), 365 (11)	2, 3,3-DMA on C3' A- ring and C3 B-ring	Kanzonol Y or Glycybridin C

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
G19	28.23	282, 338	C ₂₅ H ₂₆ O ₆	n.i.	421	205 (42), 403 (100)	423	203 (33), 217 (16), 219 (73), 247 (29), 321 (77), 339 (30), 349 (24), 367 (10), 377 (100), 395 (26), 405 (60)	308 (40), 309 (17), 321 (88), 349 (100)	1 or 2, 3,3-DMA, n.i.	n.i. At least single 3,3- DMA prenylated
G20	28.74	362	C ₂₅ H ₂₆ O ₆	n.i.	421	393 (100)	423	177 (10), 191 (62), 203 (75), 219 (100), 339 (10), 355 (11), 377 (31), 395 (15)	191 (100)	0	n.i. Not prenylated
G-I-21	28.93	342	C ₂₅ H ₂₆ O ₄	Flavone	389	334 (100), 335 (18), 389 (29), 390 (13)	391	335 (100)	149 (19), 279 (100)	2, 3,3-DMA on C6 A- ring and C3' B-ring	Licoflavone B
G22	29.30	<u>278</u> , 358	C ₂₁ H ₂₂ O ₅	Isoflavan	353	150 (16), 165 (41), 175 (28), 201 (100), 321 (19), 338 (41)	355	153 (84), 189 (100)	147 (100), 171 (18)	1, 2,2-DMP, C8 A-ring	3'-Hydroxy-4'- methoxyglabridin
G-I-23	29.53	<u>282</u> , 318	C ₂₅ H ₂₈ O ₄	Flavanone	391	187 (23), 203 (100)	393	205 (13), 337 (100)	177 (27), 191 (16), 195 (52), 203 (17), 213 (100), 281 (19), 295 (22), 319 (63), 322 (27)	2, 3,3-DMA, C8 A-ring and C3' B-ring	Glabrol
G24	30.89	286, 334	C ₂₅ H ₃₀ O ₅	2'-hydroxy- dihydrochalcone	409	217 (19), 235 (100), 391 (30)	411	179 (11), 337 (68), 355 (7), 365 (27), 393 (100)	175 (17), 337 (100)	2, 3,3-DMA on C3' A- ring and C3 B-ring	Kanzonol Y or Glycybridin C
G25	31.29	350	C ₂₅ H ₂₆ O ₅	3-Arylcoumarin	405	229 (10), 281 (12), 293 (100), 307 (28), 336 (93), 337 (12), 349 (39), 350 (25), 361 (52), 362 (42), 377 (18), 405 (21)	407	351 (100)	295 (100)	2, 3,3-DMA on C8 A- ring and C3' B-ring	Licocoumarin A
G-I-26	31.76	<u>282</u> , 342	C ₂₅ H ₂₈ O ₆	Isoflavan	423	193 (55), 229 (100), 391 (24)	425	313 (12), 369 (100)	189 (45), 191 (13), 313 (100), 351 (48)	2, 3,3-DMA on C8 A- ring and C3' B-ring	Gancaonin E
G27	31.76	<u>282</u> , 342	C ₂₅ H ₃₀ O ₄	Isoflavan	393	n.d.	395	135 (10), 191(100), 339 (49)	135 (100)	2, 3,3-DMA on C8 A- ring and C3' B-ring	Kanzonol X
G28	33.18	<u>278</u> , 358	C ₂₁ H ₂₂ O ₄	Isoflavan	337	123 (10), 175 (56), 201 (100), 213 (11), 322 (48)	339	137 (66), 189 (100)	147 (100), 171 (21)	1, 2,2-DMP on C8 A-ring	4'-Methoxyglabridin
G29	33.89	294, <u>330</u>	C ₂₅ H ₂₄ O ₄	Flavone	387	n.d.	389	333 (100), 334 (26), 347 (10), 389 (24)	249 (10), 263 (31), 277 (45), 279 (37), 287 (17), 290 (17), 291 (46), 304 (12), 305 (100), 306 (17), 315 (31), 318 (62), 319 (32), 333 (19)	2, 3,3-DMA on C6 A- ring and 2,2-DMP on C3' B-ring	Kanzonol E isomer
G30	34.48	278, <u>342</u>	C ₂₄ H ₂₈ O ₅	n.i.	395	177 (12), 217 (100)	397	179 (46), 191 (52), 341 (100), 379 (14)	189 (21), 191 (30), 267 (15), 285 (100),	2, 3,3-DMA, n.i.	n.i. Double 3,3-DMA prenylated

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
G31	35.18	<u>282</u> , 354	C ₂₅ H ₂₈ O ₄	Isoflavan	391	n.d.	393	189 (84), 191 (66), 201 (11), 337 (100)	313 (15), 323 (32) 123 (10), 137 (23), 161 (26), 173 (12), 175 (30), 177 (13), 187 (22), 189 (62), 201 (100), 203 (19), 213 (37), 215 (31), 277 (10), 319 (36)	2, 3,3-DMA on C8 A- ring and 2,2-DMP on C3' B-ring	8-Prenylphaseollin isoflavan
G32	36.00	274, 354	n.i.	n.i.	659	335 (100)	661	337 (13), 351 (68), 441 (20), 593 (15), 605 (100), 643 (31)	307 (20), 549 (36), 587 (100)	2, 3,3-DMA, n.i.	n.i. Double 3,3-DMA prenylated
G33	37.67	<u>278</u> , 330	C ₂₅ H ₂₈ O ₄	Isoflavan	391	175 (15), 177 (50), 187 (16), 188 (11), 189 (36), 201 (50), 203 (100), 213 (20), 322 (30), 323 (10), 335 (15), 347 (29), 373 (12)	393	191 (72), 337 (100)	149 (23), 161 (16), 173 (12), 177 (10), 187 (37), 189 (100), 201 (32), 203 (22), 295 (22), 319 (10)	2, 2,2-DMP on C8 A- ring and 3,3-DMA on C3' B-ring	Hispaglabridin A
G35	39.34	382	C ₂₅ H ₂₈ O ₅	Chalcone	407	203 (100)	409	205 (21), 335 (23), 353 (100)	177 (13), 211 (18), 229 (36), 297 (8), 311 (2), 335 (100)	2, 3,3-DMA on C3' A- ring and C3 B-ring	Glyinflanin A
G36	39.53	282, <u>326</u>	C ₂₄ H ₂₄ O ₄	n.i.	375	319(100), 320 (26), 331 (62), 332 (22), 357 (10)	377	308 (16), 309 (11), 320 (15), 321 (34), 348 (11), 349 (53), 361 (100), 352 (28)	293 (15), 305 (100), 306 (27), 333 (18), 361 (16)	1, 3,3-DMA on C3' B- ring	n.i. Single 3,3-DMA prenylated on C3' B-ring
G37	39.53	282, <u>326</u>	C ₃₀ H ₄₄ O ₄	Triterpenoid	467	423 (100)	469	175 (12), 189 (27), 205 (14), 217 (28), 233 (13), 235 (12), 317 (11), 405 (32), 423 (100), 451 (41)	217 (55), 405 (100) ^(e)	0	3-Oxoglycyrrhithenic acid
G38	42.03	<u>274</u> , 350	C ₂₅ H ₂₄ O ₄	n.i.	387	173 (12), 175 (34), 199 (13), 211 (16), 317 (11), 318 (29), 319 (12), 332 (12), 343 (20), 344 (16), 357 (17), 359 (20), 369 (34), 371 (17), 372 (100), 373(11), 387 (13)	389	159 (13), 187 (27), 211 (26), 213 (15), 317 (61), 318 (10), 331 (17), 345 (79), 346 (13), 355 (11), 357 (21), 359 (18), 369 (58), 370 (12), 371 (30), 372 (100), 373 (15), 387 (79), 388 (48)	329 (20), 343 (13), 344 (11), 355 (11), 356 (17), 357 (100), 371 (43)	1 or 2, 2,2-DMP, n.i.	n.i. At least single 2,2- DMP prenylated
G39	42.68	278	C ₂₅ H ₂₆ O ₄	Isoflavan	389	349 (100), 389 (13)	391	147 (8), 189 (100)	147 (100), 171 (22)	2, 2,2-DMP on C8 A-ring and C3' B-ring	Hispaglabridin B
G40	44.32	346	C ₃₀ H ₄₆ O ₂	n.i.	455 ^(d)	387 (100) ^(e)	439	241 (13), 259 (17), 269 (12), 287 (14), 393 (100)	157 (10), 171 (31), 185 (34), 199 (28), 201 (12), 213 (23),	0	n.i. Not prenylated

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
G41	44.89	346	n.i.	n.i.	711	335 (100), 375 (24), 377 (11), 387 (38), 521 (64), 533 (70)	713	333 (11), 387 (23), 389 (40), 537 (42), 657 (100), 370 (29), 698 (14)	215 (16), 225 (13), 227 (19), 240 (16), 241 (100), 243 (11), 255 (64), 257 (12), 269 (96), 283 (23), 323 (17), 337 (16) 333 (35), 335 (11), 385 (19), 399 (20), 453 (12), 467 (11), 469 (14), 481 (59), 482 (15), 521 (13), 523 (11), 601 (100), 639 (41)	2, 3,3-DMA, n.i.	n.i. Double chain prenylated
<i>G. inflata</i>											
I-U-4	6.16	<u>290</u> , 330	C ₁₅ H ₁₂ O ₅	Flavanone	271	151 (100), 177 (22)	273	147 (98), 153 (100)	67 (83), 111 (100)	0	Naringenin
I-U-6	6.16	370	C ₁₆ H ₁₄ O ₄	Chalcone	269	149 (13), 175 (62), 237 (100)	271	229 (100), 271 (38)	107 (40), 123 (100)	0	Echinatin
I7	16.04	262 ^{sh} , 283, 330	C ₂₀ H ₁₆ O ₆	Isoflavone	351	283 (100), 307 (10)	353	299 (24), 311 (100), 325 (31), 335 (22)	153 (28), 255 (60), 283 (100), 293 (13), 311 (58)	1, 2,2-DMP, C3' B-ring	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B
I-U-8	16.21	<u>286</u> , 342	C ₂₀ H ₁₈ O ₆	Isoflavanone	353	125 (57), 165 (13), 227 (100)	355	151 (35), 179 (37), 189 (100), 201 (12), 229 (61), 313 (20), 327 (48), 337 (63)	147(100), 161 (11), 171 (26)	1, 2,2-DMP, C3' B-ring	Licoisoflavanone
I10	17.63	<u>286</u> , 342	C ₂₀ H ₂₀ O ₆	n.i.	355	125 (20), 229 (100)	357	301 (100)	123 (16), 147 (14), 175 (93), 273 (12), 283 (100)	1, 3,3-DMA, n.i.	n.i. A-ring 3,3-DMA prenylated without <i>ortho</i> -OCH ₃
I-U-12	17.79	<u>262</u> , 326	C ₂₀ H ₁₆ O ₆	Isoflavone	351	177 (11), 293 (10), 295 (15), 308 (12), 323 (26), 333 (100), 334 (14), 336 (57), 351 (13)	353	153 (46), 201 (7), 227 (17), 297 (12), 307 (39), 311 (18), 325 (15), 335 (100)	153 (15), 281 (12), 307 (100), 317 (15), 320 (20), 335 (20)	1, 2,2-DMP, C3' B-ring	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B
I13	18.25	270, <u>346</u>	C ₂₀ H ₁₈ O ₅	Flavone	337	268 (100), 281 (50), 282 (24), 337 (45)	339	283 (100)	213 (89), 241 (23), 255 (24), 283 (100)	1, 3,3-DMA, C8 A-ring	Licoflavone C
I-U-14	19.11	<u>278</u> , 370	C ₂₁ H ₂₄ O ₅	Isoflavan	355	207 (17), 219 (15), 233 (17), 245 (14), 254 (12), 286 (10)	357	221 (48), 235 (36), 289 (6), 301 (100)	137 (8), 165 (59), 179 (100), 191 (15), 269 (13), 283 (18)	1, 3,3-DMA, C6 A-ring	Glyasperin C
I-U-15	20.46	<u>286</u> , 346	C ₂₀ H ₁₈ O ₆	Isoflavanone	353	125 (100)	355	151 (53), 179 (48), 189 (97), 201 (17), 229 (70), 298 (16), 299 (19), 313 (14), 327 (39), 337 (100)	253 (18), 267 (19), 281 (24), 291 (14), 295 (100), 309 (66), 319 (82), 322 (31)	1, 3,3-DMA, C3' B-ring	Uralenin
I-U-16	20.75	<u>262</u> , 334	C ₂₀ H ₁₈ O ₆	Isoflavone	353	267 (15), 284 (59), 285 (100)	355	287 (<1), 299(100)	147 (63), 173 (19), 191 (27), 217 (43),	1, 3,3-DMA, C3' B-ring	Licoisoflavone A

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
I17	21.90	314, <u>378</u>	C ₂₁ H ₂₂ O ₄	Chalcone	337	229 (10), 243 (53), 268 (43), 305 (100), 306 (13), 307 (15)	339	219 (10), 245 (21), 271 (30), 297 (100)	229 (11), 243 (67), 245 (51), 253 (35), 271(100), 281 (30), 299 (13)	1, 1,1-DMA, C3 B-ring	Licochalcone A
I-U-18	22.55	350	C ₂₀ H ₁₈ O ₅	Isoflavone	337	273 (37), 268 (11), 281 (100), 282 (25), 293 (16), 294 (12), 305 (19), 337 (98), 338 (19)	339	203 (12), 271 (21), 283 (100), 297 (16)	191 (100), 203 (31), 227 (27), 229 (17), 237 (17), 241 (11), 255 (21), 265 (22)	1, 3,3-DMA, C3' B-ring	3'-Prenylgenistein (isowighteone)
I-U-19	22.55	350	C ₂₁ H ₁₈ O ₆	Coumestan	365	295 (45), 307 (100), 349 (13), 350 (20)	367	283 (14), 311 (100), 339 (25)	281 (100), 283 (24), 295 (42)	1, 3,3-DMA, C6 A-ring	Glycyrol
I-U-20	25.52	262	C ₂₀ H ₁₆ O ₆	Isoflavone	351	265 (11), 283 (100)	353	299 (20), 311 (100), 325 (30), 335 (22)	153 (24), 255 (58), 283 (100), 284 (10), 293 (12),311 (54)	1, 2,2-DMP, C3' B-ring	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B
I22	27.63	262 ^{sh} , 330	C ₂₀ H ₁₆ O ₅	Isoflavone	335	305 (19), 307 (14), 317 (56), 320 (100), 321 (15), 335 (84), 336 (14)	337	153 (100), 211 (39), 295 (74), 309 (24), 319 (68)	n.d.	1, 2,2-DMP, C3' B-ring	Isoderrone
I-U-24	30.33	282	C ₂₂ H ₂₆ O ₅	Isoflavan	369	135 (25), 147 (26), 221 (17), 337 (100), 339 (12)	371	167 (6), 235 (15), 301 (15), 303 (87), 315 (100)	179 (50), 193 (100), 297 (9)	1, 3,3-DMA, C6 A-ring	Glyasperin D
I25	30.78	<u>286</u> , 330	C ₂₅ H ₂₈ O ₅	Flavanone	407	185 (12), 229 (19), 245 (100)	409	189 (34), 205 (100), 231 (15), 353 (66)	149 (100)	2, 3,3-DMA, C6 A-ring and C3' B-ring	Macarangaflavanone B (Paratocarpin L)
I27	32.55	<u>294</u> , 346	C ₂₅ H ₂₈ O ₅	n.i.	407	219 (100), 245 (12)	409	353 (100)	161 (11), 165 (23), 167 (25), 189 (15), 191 (38), 193 (100), 195 (16), 213 (40), 219 (32), 297 (15), 311 (24), 335 (10)	2, 3,3-DMA and 2,2- DMP, n.i.	n.i. Double 3,3-DMA and 2,2-DMP prenylated
I28	33.46	267 ^{sh} , 358	C ₂₅ H ₂₆ O ₆	n.i.	421	335 (28), 352 (100), 353 (45), 377 (10)	423	367 (100)	165 (19), 219 (60), 311 (100)	2, 3,3-DMA, n.i.	n.i. Double 3,3-DMA prenylated
I29	34.14	<u>294</u> , 346	C ₂₅ H ₂₈ O ₆	Flavanone	423	193 (91), 229 (100)	425	369 (100)	189 (19), 191(100), 313 (4), 351 (12)	2, 3,3-DMA, C8 A-ring and C3' B-ring	Gancaonin E isomer
I-U-30	34.81	<u>266</u> , 342	C ₂₅ H ₂₆ O ₆	Isoflavone	421	309 (13), 352 (53), 365 (51), 366 (100), 367 (13), 392 (15), 421 (29), 422 (16)	423	367 (100)	299 (12), 311 (100)	2, 3,3-DMA, C6 A-ring and C3' B-ring	2'-Hydroxy- Isolupalbingenin ((Iso)angustone A)
I31	36.04	274	C ₂₅ H ₂₆ O ₅	n.i.	405	183 (25), 201 (12), 227 (30), 245 (100)	407	187 (64), 205 (100), 229 (28), 351 (75)	149 (100), 163 (10)	2, 3,3-DMA, n.i.	n.i. Double 3,3-DMA prenylated

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
I32	36.45	378	C ₂₅ H ₂₆ O ₄	Flavanone	389	185 (42), 203 (100), 371 (14)	391	205 (11), 335 (100)	149 (100), 187 (50), 199 (11), 293 (3), 317 (12)	2, 3,3-DMA on C8 A-ring and 2,2-DMP C3' B-ring	Euchrenone A5
I33	36.66	<u>290</u> , 350	C ₂₅ H ₂₆ O ₆	Isoflavone	421	193 (100)	423	189 (7), 349 (20), 367 (100), 405 (46)	189 (15), 349 (100)	2, 3,3-DMA, C8 A-ring and C3' B-ring	Glyurallin B
I-U-34	38.31	<u>278</u> , 346	C ₂₅ H ₂₆ O ₅	Isoflavone	405	295 (11), 307 (46), 350 (100), 351 (10), 405 (39), 406 (16)	407	295 (6), 351 (100)	295 (100)	2, 3,3-DMA, C6 and C8 A-ring	6,8-Diprenylgenistein
I35	38.31	<u>278</u> , 346	C ₂₅ H ₂₆ O ₆	Isoflavone	421	219 (21), 267 (17), 269 (12), 309 (12), 335 (15), 352 (100), 353 (26), 377 (20), 393 (11)	423	367 (100)	311 (100)	2, 3,3-DMA, C6 A-ring and C3' B-ring	2'-Hydroxy- isolupalbingenin (Iso)angustone A)
I36	42.31	<u>266</u> , 346	C ₂₅ H ₂₄ O ₆	Isoflavone	419	219 (42), 265 (52), 267 (40), 333 (34), 350 (26), 351 (47), 375 (100), 376 (21), 391 (20), 401 (30), 404 (44)	421	365 (100)	165 (100), 201 (31), 323 (5), 347 (34)	2, 3,3-DMA on C6 A-ring and 2,2-DMP C3' B-ring	Angustone B
<i>G. uralensis</i>											
U5	13.48	286	C ₂₁ H ₂₂ O ₆	Isoflavanone	369	229 (100)	371	315 (100)	141 (23), 147 (17), 153 (38), 175 (100), 193 (25), 287 (10), 297 (68)	1, 3,3-DMA, C6 A-ring	Glyasperin B
U7	21.97	370	C ₂₁ H ₂₂ O ₅	Chalcone	353	297 (100), 298 (21), 310 (12), 353 (49)	355	287 (100), 299 (70)	165 (13), 231 (11), 241 (14), 287 (100)	1, O-3,3-DMA, n.i.	n.i. O-3,3-DMA prenylated
U9	18.50	350	C ₂₁ H ₂₀ O ₆	3-Arylcoumarin	367	284 (12), 297 (38), 309 (100), 352 (15)	369	285 (45), 301 (5), 313 (100), 314 (13), 327 (14), 341 (11)	149 (19), 191 (19), 209 (11), 243 (17), 257 (10), 271 (27), 281 (23), 283 (32), 285 (100), 298 (14)	1, 3,3-DMA, C6 A-ring	Glycycoumarin
U10	19.78	<u>268</u> , 330	C ₂₀ H ₁₈ O ₆	Isoflavone	353	284 (44), 297 (56), 298 (100)	355	287 (39), 299 (100)	243 (35), 271 (100)	1, 3,3-DMA, C3' B-ring	Glycyrrhisoflavone
U11	21.00	286, <u>322</u>	C ₂₁ H ₂₂ O ₅	n.i.	353	177 (19), 270 (17), 283 (30), 284 (41), 285 (69), 295 (23), 321 (51), 338 (100)	355	221 (26), 299 (100)	177 (100) ^(c)	1, 3,3-DMA, C6 A-ring	n.i. C6 3,3-DMA prenylated without <i>ortho</i> -OCH ₃
U13	21.97	<u>286</u> , 370	C ₂₂ H ₂₂ O ₆	Isoflavone	381	311 (15), 323 (99), 324 (11), 351 (100), 352 (12), 367 (9)	383	178 (15), 191 (21), 257 (12), 295 (20), 299 (100), 312 (18), 315 (<1)	178 (10), 191 (16), 257 (10), 295 (20), 299 (100), 312 (21)	1, 3,3-DMA, C3' B-ring	Licoricone
U17	25.90	<u>274</u> , 318	C ₂₁ H ₂₄ O ₆	n.i.	371	261 (100)	373	305 (39), 317 (100), 318 (10), 332 (24), 333 (10), 344 (16),	207 (100)	1, 3,3-DMA, B-ring	n.i. B-ring 3,3-DMA prenylated

No.	Rt (min)	UV _{max} (nm) ^(a)	Molecular formula	Class	[M-H] ⁻ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	MS ³ PI mode <i>m/z</i> (R.A.)	Prenyl number, configuration ^(b) , and position	Tentatively identified compound
U21	27.38	350	C ₂₂ H ₂₂ O ₆	3-Arylcoumarin	381	337 (27), 350 (12), 351 (53), 352 (53), 353 (16), 365 (42), 366 (100)	383	346 (18), 353 (11), 355 (16), 357 (25), 364 (13) 299 (100), 300 (18), 315 (3), 327 (21), 341 (7)	239 (13), 243 (43), 257 (12), 271 (23), 284 (100), 285 (9), 299 (23)	1, 3,3-DMA, C6 A-ring	Glycyrin
U22	31.83	<u>282</u> , 338	C ₂₆ H ₃₂ O ₅	Isoflavan	423	193 (55), 229 (100), 391 (24)	425	191 (11), 221 (19), 369 (100)	167 (85), 189 (100), 191 (17), 219 (17), 233 (17), 313 (45), 351 (13)	2, 3,3-DMA, C6 A-ring and C3' B-ring	Licoricidin
U23	32.11	334	C ₂₂ H ₂₄ O ₅	Isoflav-3-ene	367	297 (15), 309 (62), 337 (100), 352 (75)	368 ^(c)	167 (9), 191 (11), 215 (11), 259 (19), 299 (20), 300 (42), 301 (32), 312 (13), 313 (100), 337 (10), 353 (62), 354 (41), 368 (19)	107 (26), 175 (16), 179 (21), 191 (49), 203 (63), 204 (15), 239 (13), 253 (28), 263 (16), 281 (47), 283 (31), 285 (29), 294 (14), 295 (53), 296 (26), 297 (19), 298 (100), 311 (17)	1, 3,3-DMA, C6 A-ring	Dehydroglyasperin D
U25	33.53	282, <u>322</u>	C ₂₅ H ₂₆ O ₆	Flavonol	421	309 (11), 323 (52), 335 (12), 352 (40), 353 (55), 366 (100), 377 (10), 392 (14), 393 (14), 421 (50), 422 (27)	423	311 (6), 367 (100)	311 (100)	2, 3,3-DMA, C6 A-ring and C3' B-ring	Glyasperin A
U26	35.25	<u>290</u> , 346	C ₂₆ H ₃₀ O ₅	Pterocarpan	421	338 (22), 351 (43), 352 (14), 363 (34), 365 (11), 366 (12), 377 (15), 389 (76), 406 (100)	423	191 (11), 221 (18), 367 (100)	191 (10), 299 (19), 311 (100)	2, 3,3-DMA, C6 A-ring and C3' B-ring	1-Methoxyficifolinol
U27	35.44	342	C ₂₁ H ₂₀ O ₅	Isoflavone	n.d.	n.d.	353	297 (100)	267 (100)	1, 3,3-DMA, C6 A-ring	Gancaonin A
U28	36.04	274, 342	C ₂₂ H ₂₄ O ₆	n.i.	383	207 (100)	385	311 (8), 329 (100), 367 (21)	311 (100)	1, 3,3-DMA, n.i.	n.i. C6 3,3-DMA prenylated without <i>ortho</i> -OCH ₃
U29	36.81	338	n.d.	n.i.	775	435 (10), 555 (100), 567 (82)	777	513 (15), 269 (22), 665 (13), 720 (16), 721 (100)	513 (19), 555 (11), 611 (11), 665 (100)	2, 3,3-DMA, n.i.	n.i. double 3,3-DMA prenylated
U31	41.84	<u>282</u> , 342	C ₂₇ H ₃₄ O ₅	Isoflavan	437	177 (21), 203 (54), 215 (54), 221 (16), 405 (100), 406 (23)	439	371 (47), 383 (100)	181 (100), 189 (86), 191 (20), 193 (15), 215 (12), 327 (58)	2, 3,3-DMA, C6 A-ring and C3' B-ring	Licorisoflavan A

n.d. Not detected; n.i. Not identified; ^{sh} Shoulder; R.A. Relative abundance.

^(a)Underlined numbers indicate the main UV absorbance peak.

^(b)3,3-DMA = 3,3-dimethyl chain; 1,1-DMA = 1,1-dimethylallyl chain; 2,2-DMP = 2,2-dimethylpyran ring.

^(c)[M]⁺ instead of [M+H]⁺.

^(d)Water adduct seen in full MS.

^(e)Only fragments with a R.A. > 50 % are shown.

F. Tentative identification of prenylated phenolics in EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent by FT-MSⁿ

Table F1. Tentative identification of prenylated phenolics in EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent (**Figure 2**) and the spectrometric data obtained using negative and positive ionisation (PI) mode ESI-FT-MSⁿ. Numbers refer to peaks in **Figure 2**. Bold number indicate the same compound between *Glycyrrhiza* species (G = *G. glabra*, I = *G. inflata*, and U = *G. uralensis*). MSⁿ spectra of *G. glabra* adapted from ².

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound		
<i>G. glabra</i>								
G-I-U-1	C ₁₅ H ₁₂ O ₄ (-0.099)	255.06619	91.01920 – C ₆ H ₃ O [•] (15), 119.05018 – C ₈ H ₇ O [•] (100)	257.08081	81.03410 – C ₅ H ₅ O ⁺ (26), 91.05473 (21), 119.04931 – C ₈ H ₇ O ⁺ (30),	Liquiritigenin		
G-I-U-2	C ₁₅ H ₁₂ O ₄ (-0.099)	255.06633	91.01920 - C ₆ H ₃ O [•] (28), 119.05018 - C ₈ H ₇ O [•] (100),	257.08096	81.03365 - C ₅ H ₅ O ⁺ (26), 91.05436, 119.04934 - C ₈ H ₇ O ⁺ (29), 137.02354 - C ₇ H ₅ O ₃ ⁺ (100),	Isoliquiritigenin		
G-I-U-3	C ₁₆ H ₁₂ O ₄ (0.129)	267	91.01922 - C ₆ H ₃ O [•] (15), 132.02165 - C ₈ H ₄ O ₂ [•] (68), 135.00876 - C ₇ H ₃ O ₃ [•] (12), 153.01930 - C ₇ H ₃ O ₄ [•] (18), 195.04498 - C ₁₃ H ₇ O ₂ [•] (47), 208.05280 - C ₁₄ H ₈ O ₂ [•] (16)	223.03995 - C ₁₄ H ₇ O ₃ [•] (100), 224.04608 (19), 251.03481 - C ₁₅ H ₇ O ₄ [•] (51), 252.04271 - C ₁₅ H ₈ O ₄ [•] (62), 253.04585 (12)	269.08087	107.04928 - C ₇ H ₇ O ⁺ (24), 108.02074 - C ₆ H ₄ O ₂ ⁺ (13), 118.04143 - C ₈ H ₆ O ⁺ (83), 133.06497 - C ₉ H ₉ O ⁺ (15), 137.02350 - C ₇ H ₅ O ₃ ⁺ (31), 154.02620 - C ₇ H ₆ O ₄ ⁺ (27), 156.05710 - C ₁₁ H ₈ O ⁺ (19), 170.07300 - C ₁₂ H ₁₀ O ⁺ (23), 181.06503 - C ₁₃ H ₉ O ⁺ (35), 182.07358 (17), 121.02859 – C ₇ H ₅ O ₂ ⁺ (17), 149.02332 – C ₈ H ₅ O ₃ ⁺ (12), 167.03383 – C ₈ H ₇ O ₄ ⁺ (49), 211.07515 – C ₁₄ H ₁₁ O ₂ ⁺ (10),	197.05997 - C ₁₃ H ₉ O ₂ ⁺ (100), 198.06744 - C ₁₃ H ₁₀ O ₂ ⁺ (33), 213.09122 - C ₁₄ H ₁₃ O ₂ ⁺ (57), 225.05478 - C ₁₄ H ₉ O ₃ ⁺ (43), 226.06274 - C ₁₄ H ₁₀ O ₃ ⁺ (84), 237.05479 - C ₁₅ H ₉ O ₃ ⁺ (70), 238.05811 (14), 253.04977 - C ₁₅ H ₉ O ₄ ⁺ (95), 254.05727 - C ₁₅ H ₁₀ O ₄ ⁺ (42), 269.08109 - C ₁₆ H ₁₃ O ₄ ⁺ (33)	Formononetin
G4	C ₂₀ H ₁₈ O ₄ (-0.017)	321.11301	99.92966 (11), 102.94907 (26), 116.92850 (12), 117.03457 - C ₈ H ₅ O [•] (57), 118.96619 (34), 123.94941 (11), 146.96115 (100),	265.05008 - C ₁₆ H ₉ O ₄ [•] (12), 266.05820 - C ₁₆ H ₁₀ O ₄ [•] (55), 267.06180 (13), 298.04813 - C ₁₆ H ₁₀ O ₆ [•] (29)	323.12778	239.07013 – C ₁₅ H ₁₁ O ₃ ⁺ (21), 240.07784 – C ₁₅ H ₁₂ O ₃ ⁺ (11), 267.06497 – C ₁₆ H ₁₁ O ₄ ⁺ (100), 268.07065 – C ₁₆ H ₁₂ O ₄ ⁺ (29)	7,4'-Dihydroxy-8-prenylflavone	

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound	
			237.05554 - C ₁₅ H ₉ O ₃ ⁻ (12),				
G-I-5	C ₂₀ H ₁₈ O ₄ (2.242)	321.11316	79.05543 - C ₆ H ₇ ⁻ (32), 99.92620 (11), 102.94905 (35), 105.07108 - C ₈ H ₉ ⁻ (21), 107.05037 (86), 109.02943 - C ₆ H ₅ O ₂ ⁻ (15), 116.92857 (18), 117.03456 - C ₈ H ₅ O ⁻ (17), 118.96621 (34), 121.02946 - C ₇ H ₅ O ₂ ⁻ (16),	133.02950 - C ₈ H ₅ O ₂ ⁻ (26), 145.02940 - C ₉ H ₅ O ₂ ⁻ (26), 146.96115 (100), 175.07629 - C ₁₁ H ₁₁ O ₂ ⁻ (35), 199.07626 - C ₁₃ H ₁₁ O ₂ ⁻ (29), 265.05042 - C ₁₆ H ₉ O ₄ ⁻ (15), 277.05112 - C ₁₇ H ₉ O ₄ ⁻ (12), 291.06644 - C ₁₈ H ₁₁ O ₄ ⁻ (16), 305.08173 - C ₁₉ H ₁₃ O ₄ ⁻ (14), 306.08911 - C ₁₉ H ₁₄ O ₄ ⁻ (16)	323.12772 147.04424 - C ₉ H ₇ O ₂ ⁺ (19), 147.08061 - C ₁₀ H ₁₁ O ⁺ (11), 173.06001 - C ₁₁ H ₉ O ₂ ⁺ (10), 189.09117 - C ₁₂ H ₁₃ O ₂ ⁺ (6), 267.06540 - C ₁₆ H ₁₁ O ₄ ⁺ (17), 279.06549 - C ₁₇ H ₁₁ O ₄ ⁺ (100),	280.06891 (31), 307.09683 - C ₁₉ H ₁₅ O ₄ ⁺ (29)	Glabrene
G6	C ₂₀ H ₂₀ O ₄ (0.259)	323.12894	n.d.	325.14368	77.00566 (19), 105.00065 (15), 123.04418 - C ₇ H ₇ O ₂ ⁺ (100), 147.04430 - C ₉ H ₇ O ₂ ⁺ (15),	147.08055 - C ₁₀ H ₁₁ O ⁺ (23), 189.09122 - C ₁₂ H ₁₃ O ₂ ⁺ (13)	Phaseollinisoflavan
G7	C ₁₉ H ₁₆ O ₄ (-0.488)	n.d.	n.d.	308.10416 ^(e)	210.92195 (13), 265.08615 - C ₁₇ H ₁₃ O ₃ ⁺ (28),	293.08102 - C ₁₈ H ₁₃ O ₄ ⁺ (100), 294.08447 (24)	n.i. Not prenylated
G8	C ₂₀ H ₁₆ O ₅ (-0.178)	335.09250	91.01919 - C ₆ H ₃ O ⁻ (62), 93.03488 - C ₆ H ₅ O ⁻ (44), 107.05038 - C ₇ H ₇ O ⁻ (38), 135.00873 - C ₇ H ₅ O ₃ ⁻ (70), 153.01921 - C ₇ H ₅ O ₄ ⁻ (54), 183.04521 - C ₁₂ H ₇ O ₂ ⁻ (30), 199.07628 - C ₁₃ H ₁₁ O ₂ ⁻ (73), 213.05540 - C ₁₃ H ₉ O ₃ ⁻ (21), 227.03477 - C ₁₃ H ₇ O ₄ ⁻ (23), 231.08115 - C ₁₁ H ₁₁ O ⁻ (23),	243.87976 (28), 261.89026 (44), 273.09213 - C ₁₉ H ₁₃ O ₂ ⁻ (21), 291.10254 - C ₁₉ H ₁₅ O ₃ ⁻ (100), 292.10565 (23), 305.04535 - C ₁₈ H ₉ O ₅ ⁻ (47), 319.06085 - C ₁₉ H ₁₁ O ₅ ⁻ (37), 320.06845 - C ₁₉ H ₁₂ O ₅ ⁻ (24), 335.09253 - C ₂₀ H ₁₅ O ₅ ⁻ (71), 336.09534 (19)	337.10706 79.05431 - C ₆ H ₇ ⁻ (11), 81.07001 - C ₆ H ₉ ⁻ (37), 109.06502 - C ₇ H ₉ O ⁺ (29), 137.02354 - C ₇ H ₅ O ₃ ⁺ (100), 147.04410 - C ₉ H ₇ O ₂ ⁺ (10), 193.04976 - C ₁₀ H ₉ O ₄ ⁺ (13), 201.05487 - C ₁₂ H ₉ O ₃ ⁺ (38), 229.04951 - C ₁₃ H ₉ O ₄ ⁺ (12), 239.07051 - C ₁₅ H ₁₁ O ₃ ⁺ (37), 255.06580 - C ₁₅ H ₁₁ O ₄ ⁺ (15),	266.05771 - C ₁₆ H ₁₀ O ₄ ⁺ (10), 267.06549 - C ₁₆ H ₁₁ O ₄ ⁺ (47), 268.06888 (10), 283.06036 - C ₁₆ H ₁₁ O ₅ ⁺ (47), 284.06387 (10), 295.06052 - C ₁₇ H ₁₁ O ₅ ⁺ (83), 296.06406 (16), 319.09671 - C ₂₀ H ₁₅ O ₄ ⁺ (15), 337.10721 - C ₂₀ H ₁₇ O ₅ ⁺ (18),	Glabrone
G-I-9	C ₂₀ H ₁₆ O ₅ (-0.178)	335.09271	91.01919 - C ₆ H ₃ O ⁻ (62), 93.03488 - C ₆ H ₅ O ⁻ (44), 107.05038 - C ₇ H ₇ O ⁻ (38), 135.00873 - C ₇ H ₇ O ₃ ⁻ (70), 153.01921 - C ₇ H ₅ O ₄ ⁻ (54), 183.04521 - C ₁₂ H ₇ O ₂ ⁻ (30), 199.07628 - C ₁₃ H ₁₁ O ₂ ⁻ (74), 213.05540 - C ₁₃ H ₉ O ₃ ⁻ (21), 227.03477 - C ₁₃ H ₇ O ₄ ⁻ (23), 231.08115 - C ₁₇ H ₁₁ O ⁻ (23),	243.87976 (28), 261.89026 (44), 273.09213 - C ₁₉ H ₁₃ O ₂ ⁻ (20), 291.10254 - C ₁₉ H ₁₅ O ₃ ⁻ (100), 292.10565 (23), 305.04535 - C ₁₈ H ₉ O ₅ ⁻ (47), 319.06085 - C ₁₉ H ₁₁ O ₅ ⁻ (37), 320.06845 - C ₁₉ H ₁₂ O ₅ ⁻ (24), 335.09253 - C ₂₀ H ₁₅ O ₅ ⁻ (71), 336.09534 (19)	337.10699 81.07067 - C ₆ H ₉ ⁺ (38), 109.06530 - C ₇ H ₉ O ⁺ (28), 137.02356 - C ₇ H ₅ O ₃ ⁺ (100), 193.05006 - C ₁₀ H ₉ O ₄ ⁺ (15), 201.05486 - C ₁₂ H ₉ O ₃ ⁺ (42), 229.04974 - C ₁₃ H ₉ O ₄ ⁺ (13), 239.07048 - C ₁₅ H ₁₁ O ₃ ⁺ (44), 255.06583 - C ₁₅ H ₁₁ O ₄ ⁺ (14),	267.06540 - C ₁₆ H ₁₁ O ₄ ⁺ (44), 283.06036 - C ₁₆ H ₁₁ O ₅ ⁺ (67), 295.06049 - C ₁₇ H ₁₁ O ₅ ⁺ (91), 296.06357 (26), 319.09729 - C ₂₀ H ₁₅ O ₄ ⁺ (19), 321.08593 (12), 322.08270 - C ₁₉ H ₁₄ O ₅ ⁺ (11), 337.10742 - C ₂₀ H ₁₇ O ₅ ⁺ (32)	Glabrocoumarin
G10	C ₂₁ H ₂₂ O ₅ (0.224)	353.08112	108.02187 - C ₆ H ₄ O ₂ ⁻ (14), 109.06584 - C ₇ H ₉ O ⁻ (15), 121.02947 - C ₇ H ₅ O ₂ ⁻ (25), 122.03729 - C ₇ H ₆ O ₂ ⁻ (47),	177.09195 - C ₁₁ H ₁₃ O ₂ ⁻ (100), 178.09526 (12), 181.89746 (17), 183.91296 (20)	355.15408 137.05991 - C ₈ H ₉ O ₂ ⁺ (100), 175.03922 - C ₁₀ H ₇ O ₃ ⁺ (15), 281.08112 - C ₁₇ H ₁₃ O ₄ ⁺ (23)	Licoagrochalcone C	
G-I-11	C ₂₀ H ₂₀ O ₄ (-0.263)	323.12866	91.05558 - C ₇ H ₇ ⁻ (20), 107.05035 - C ₇ H ₇ O ⁻ (38), 109.02945 - C ₆ H ₅ O ₂ ⁻ (34), 121.02948 - C ₇ H ₅ O ₂ ⁻ (13),	175.07626 - C ₁₁ H ₁₁ O ₂ ⁻ (20), 187.07642 - C ₁₂ H ₁₁ O ₂ ⁻ (12), 201.09198 - C ₁₃ H ₁₃ O ₂ ⁻ (79), 202.09529 (13),	325.14335 68.99732 - C ₃ HO ₂ ⁺ (10), 81.07001 - C ₆ H ₉ ⁺ (10), 121.06496 - C ₈ H ₉ O ⁺ (14), 123.04417 - C ₇ H ₇ O ₂ ⁺ (100),	147.08061 - C ₁₀ H ₁₁ O ⁺ (24), 149.05994 - C ₉ H ₉ O ₂ ⁺ (32), 173.05995 - C ₁₁ H ₉ O ₂ ⁺ (15), 189.09123 - C ₁₂ H ₁₃ O ₂ ⁺ (19)	Glabridin

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound
G12	C ₂₅ H ₂₈ O ₅ (0.390)	407.18628	135.04514 - C ₈ H ₇ O ₂ ⁻ (100), 136.04845 (11), 108.02184 - C ₆ H ₄ O ₂ ⁻ (12), 149.02438 - C ₈ H ₅ O ₃ ⁻ (9), 161.02432 - C ₉ H ₅ O ₃ ⁻ (31), 177.09200 - C ₁₁ H ₁₃ O ₂ ⁻ (100), 178.09528 (13), 191.10770 - C ₁₂ H ₁₅ O ₂ ⁻ (6),	213.09209 - C ₁₄ H ₁₃ O ₂ ⁻ (9), 203.07144 - C ₁₂ H ₁₁ O ₃ ⁻ (11), 221.08195 - C ₁₂ H ₁₃ O ₄ ⁻ (7), 379.19128 - C ₂₄ H ₂₇ O ₄ ⁻ (15)	409.20111 124.04758 (10), 147.04430 - C ₉ H ₇ O ₂ ⁺ (14), 69.07007 - C ₅ H ₉ ⁺ (45), 121.06490 - C ₈ H ₉ O ⁺ (10), 149.02347 - C ₈ H ₅ O ₃ ⁺ (17), 151.03903 - C ₈ H ₇ O ₃ ⁺ (12), 163.03911 - C ₉ H ₇ O ₃ ⁺ (15), 167.03410 - C ₈ H ₇ O ₄ ⁺ (100), 173.09627 - C ₁₂ H ₁₃ O ⁺ (16), 175.11177 - C ₁₂ H ₁₃ O ⁺ (7), 191.03412 - C ₁₀ H ₇ O ₄ ⁺ (9), 203.07031 - C ₁₂ H ₁₁ O ₃ ⁺ (12), 205.08609 - C ₁₂ H ₁₃ O ₃ ⁺ (12), 211.07523 - C ₁₄ H ₁₁ O ₂ ⁺ (9), 223.07593 - C ₁₄ H ₁₁ O ₂ ⁺ (13), 238.06238 - C ₁₅ H ₁₀ O ₃ ⁺ (11), 239.07059 - C ₁₅ H ₁₁ O ₃ ⁺ (9), 251.07086 - C ₁₆ H ₁₁ O ₃ ⁺ (18), 307.13923 - C ₂₀ H ₁₉ O ₃ ⁺ (22)	3-Hydroxyglabrol
G13	C ₂₀ H ₁₈ O ₄ (0.540)	321.11316	n.d.	323.12796	123.04417 - C ₇ H ₇ O ₂ ⁺ (100), 147.04425 - C ₉ H ₇ O ₂ ⁺ (8), 307.09668 - C ₁₉ H ₁₅ O ₄ ⁺ (6)	Phasecollin
G14	C ₂₁ H ₂₀ O ₅ (0.141)	351.12402	n.d.	353.13840	69.07079 - C ₅ H ₉ ⁺ (48), 153.05493 - C ₈ H ₉ O ₃ ⁺ (10), 192.91101 (14), 210.92155 (10), 213.09126 - C ₁₄ H ₁₃ O ₂ ⁺ (14), 216.87418 (12), 225.09181 - C ₁₅ H ₁₃ O ₂ ⁺ (11), 227.08069 - C ₁₄ H ₁₁ O ₃ ⁺ (15), 237.05498 - C ₁₅ H ₉ O ₃ ⁺ (22), 241.08620 - C ₁₅ H ₁₃ O ₃ ⁺ (70), 242.08945 (14), 256.07330 - C ₁₅ H ₁₂ O ₄ ⁺ (18), 260.93320 (16), 261.90186 (22), 269.08118 - C ₁₆ H ₁₃ O ₄ ⁺ (100), 270.08453 (23), 288.92819 (11), 297.07617 - C ₁₇ H ₁₃ O ₅ ⁺ (32), 297.14896 - C ₁₉ H ₂₁ O ₃ ⁺ (16)	n.i. B-ring 3,3-DMA prenylated
G15	C ₂₅ H ₂₄ O ₅ (-0.001)	n.d.	n.d.	405.16965	319.09665 - C ₂₀ H ₁₅ O ₄ ⁺ (20), 333.11240 - C ₂₁ H ₁₇ O ₄ ⁺ (19), 345.11224 - C ₂₂ H ₁₇ O ₄ ⁺ (44), 363.12292 - C ₂₂ H ₁₉ O ₅ ⁺ (45), 387.15936 - C ₂₅ H ₂₃ O ₄ ⁺ (100), 388.16272 (32), 405.17005 - C ₂₅ H ₂₅ O ₅ ⁺ (51), 406.17346 (18)	n.i. 2,2-DMP prenylated
G16	C ₂₅ H ₂₄ O ₅ (0.221)	403.15533	n.d.	405.16968	69.07076 - C ₅ H ₉ ⁺ (17), 161.02353 - C ₉ H ₅ O ₃ ⁺ (10), 203.07050 - C ₁₂ H ₁₁ O ₃ ⁺ (100), 204.07393 (13)	Scanderone
G17	C ₂₅ H ₂₄ O ₄ (0.088)	n.d.	n.d.	389.17477	147.08040 - C ₁₀ H ₁₁ O ⁺ (10), 189.09100 - C ₁₂ H ₁₃ O ₂ ⁺ (9), 279.06534 - C ₁₇ H ₁₁ O ₄ ⁺ (9), 291.06573 - C ₁₈ H ₁₁ O ₄ ⁺ (24), 305.11768 - C ₂₀ H ₁₇ O ₃ ⁺ (10), 318.08951 - C ₂₀ H ₁₄ O ₄ ⁺ (16), 319.09702 - C ₂₀ H ₁₅ O ₄ ⁺ (63), 333.11255 - C ₂₁ H ₁₇ O ₄ ⁺ (100), 334.11685 (32), 347.12817 - C ₂₂ H ₁₉ O ₄ ⁺ (32), 374.15289 - C ₂₄ H ₂₂ O ₄ ⁺ (13), 389.17532 - C ₂₅ H ₂₅ O ₄ ⁺ (83), 390.17825 (22)	Kanzonol E
G18	C ₂₅ H ₃₀ O ₅ (0.923)	409.20218	161.02434 - C ₉ H ₅ O ₃ ⁻ (14), 162.10042 (18), 174.03198 - C ₁₀ H ₆ O ₃ ⁻ (21), 177.09196 - C ₁₁ H ₁₃ O ₂ ⁻ (100), 178.09537 (15), 189.09196 - C ₁₂ H ₁₃ O ₂ ⁻ (18), 191.10757 - C ₁₂ H ₁₅ O ₂ ⁻ (11),	202.09532 (16), 216.07895 - C ₁₃ H ₁₂ O ₃ ⁻ (13), 217.08688 - C ₁₃ H ₁₃ O ₃ ⁻ (72), 235.09746 - C ₁₃ H ₁₅ O ₄ ⁻ (48), 245.08177 - C ₁₄ H ₁₃ O ₄ ⁻ (11), 246.08536 (13)	411.21698 121.06512 - C ₈ H ₉ O ⁺ (16), 123.04427 - C ₈ H ₇ O ₂ ⁺ (12), 133.02875 - C ₈ H ₅ O ₂ ⁺ (17), 133.06503 - C ₉ H ₉ O ⁺ (21), 149.02341 - C ₈ H ₅ O ₃ ⁺ (18), 149.05998 - C ₉ H ₉ O ₂ ⁺ (12), 151.03914 - C ₈ H ₇ O ₃ ⁺ (11), 175.11197 - C ₁₂ H ₁₅ O ⁺ (100), 176.11540 (19), 185.09634 - C ₁₃ H ₁₃ O ⁺ (13), 187.11205 - C ₁₃ H ₁₅ O ⁺ (18), 189.09122 - C ₁₂ H ₁₃ O ₂ ⁺ (33), 190.09454 (39), 205.08617 - C ₁₂ H ₁₃ O ₃ ⁺ (28),	Kanzonol Y or Glycybridin C

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound
G19	C ₂₅ H ₂₆ O ₆ (0.343)	421.16592	n.d.	423.18036	201.09203 - C ₁₃ H ₁₃ O ₂ ⁻ (14), 157.10153 (22), 167.03436 - C ₈ H ₇ O ₄ ⁺ (19), 173.09633 - C ₁₂ H ₁₃ O ⁺ (41), 206.08932 (14), 215.10710 - C ₁₄ H ₁₅ O ₂ ⁺ (14)	n.i. at least single 3,3-DMA prenylated
					69.07074 - C ₅ H ₉ ⁺ (12), 147.04422 - C ₉ H ₇ O ₂ ⁺ (15), 147.08069 - C ₁₀ H ₁₁ O ⁺ (15), 163.03917 - C ₉ H ₇ O ₃ ⁺ (100), 164.04250 (11), 167.03406 - C ₈ H ₇ O ₄ ⁺ (12), 175.03923 - C ₁₀ H ₇ O ₃ ⁺ (12), 181.04984 - C ₉ H ₉ O ₄ ⁺ (25), 189.09137 - C ₁₂ H ₁₃ O ₂ ⁺ (47), 203.07059 - C ₁₃ H ₁₁ O ₃ ⁺ (56), 217.08646 - C ₁₃ H ₁₃ O ₃ ⁺ (20), 219.10188 - C ₁₃ H ₁₅ O ₃ ⁺ (100), 220.10536 (13)	
G20	C ₂₅ H ₂₆ O ₆ (0.130)	421.16599	107.04860 - C ₇ H ₇ O ⁻ (10), 175.07516 - C ₁₁ H ₁₁ O ₂ ⁻ (100), 176.07852 (10), 217.08615 - C ₁₃ H ₁₃ O ₃ ⁻ (24)	423.18027	69.07081 - C ₅ H ₉ ⁺ (49), 123.0444 - C ₇ H ₇ O ₂ ⁺ (15), 135.04431 - C ₈ H ₇ O ₂ ⁺ (11), 163.03912 - C ₉ H ₇ O ₃ ⁺ (20), 173.09645 - C ₁₂ H ₁₃ O ⁺ (12), 189.09129 - C ₁₂ H ₁₃ O ₂ ⁺ (12), 149.02362 - C ₈ H ₅ O ₃ ⁺ (65), 167.03419 - C ₈ H ₇ O ₄ ⁺ (46), 279.06558 - C ₁₇ H ₁₁ O ₄ ⁺ (100), 280.06973 (24), 191.10696 - C ₁₂ H ₁₅ O ₂ ⁺ (100), 192.11029 (15), 203.07063 - C ₁₂ H ₁₁ O ₃ ⁺ (55), 281.11734 - C ₁₈ H ₁₇ O ₃ ⁺ (14), 293.08163 - C ₁₈ H ₁₃ O ₄ ⁺ (10), 309.11270 - C ₁₉ H ₁₇ O ₄ ⁺ (10)	n.i. Not prenylated
G-I-21	C ₂₅ H ₂₆ O ₄ (0.036)	389.17621	n.d.	391.19040	149.02362 - C ₈ H ₅ O ₃ ⁺ (65), 167.03419 - C ₈ H ₇ O ₄ ⁺ (46), 279.06558 - C ₁₇ H ₁₁ O ₄ ⁺ (100), 280.06973 (24), 335.12817 - C ₂₁ H ₁₉ O ₄ ⁺ (90), 336.13278 (31), 391.19092 - C ₂₅ H ₂₄ O ₄ ⁺ (15)	Licoflavone B
G22	C ₂₁ H ₂₂ O ₅ (0.140)	353.13956	102.94894 (13), 150.03214 - C ₈ H ₆ O ₃ ⁻ (78), 165.05553 - C ₉ H ₆ O ₃ ⁻ (26), 175.07610 - C ₁₁ H ₁₁ O ₂ ⁻ (19), 181.89754 (40), 183.91307 (50), 201.09207 - C ₁₃ H ₁₃ O ₂ ⁻ (100), 201.92331 (11), 202.09569 (16)	355.15405	119.04929 - C ₈ H ₇ O ⁺ (13), 147.04417 - C ₉ H ₇ O ₂ ⁺ (51), 147.08057 - C ₁₀ H ₁₁ O ⁺ (26), 153.05476 - C ₈ H ₉ O ₃ ⁺ (100), 154.05806 (12), 173.05994 - C ₁₁ H ₉ O ₂ ⁺ (12), 189.09117 - C ₁₂ H ₁₃ O ₂ ⁺ (30)	3'-Hydroxy-4'- methoxyglabridin
G-I-23	C ₂₅ H ₂₈ O ₄ (-0.117)	391.19141	132.05803 - C ₉ H ₈ O ⁻ (33), 159.08142 - C ₁₁ H ₁₁ O ⁻ (12), 164.04782 - C ₉ H ₈ O ₃ ⁻ (7), 187.11272 - C ₁₃ H ₁₅ O ⁻ (100), 188.11607 (14), 203.07130 - C ₁₂ H ₁₁ O ₃ ⁻ (17)	393.20599	133.06462 - C ₉ H ₉ O ⁺ (1), 149.02350 - C ₈ H ₅ O ₃ ⁺ (85), 167.03406 - C ₈ H ₇ O ₄ ⁺ (100), 168.03740 (8)	Glabrol
G24	C ₂₅ H ₃₀ O ₅ (0.923)	409.20218	161.02434 - C ₉ H ₅ O ₃ ⁻ (14), 162.10042 (18), 174.03198 - C ₁₀ H ₆ O ₃ ⁻ (21), 177.09196 - C ₁₁ H ₁₃ O ₂ ⁻ (100), 178.09537 (15), 189.09196 - C ₁₂ H ₁₃ O ₂ ⁻ (18), 191.10757 - C ₁₂ H ₁₅ O ₂ ⁻ (11), 201.09203 - C ₁₃ H ₁₃ O ₂ ⁻ (14), 202.09532 (16), 216.07895 - C ₁₃ H ₁₂ O ₃ ⁻ (13), 217.08688 - C ₁₃ H ₁₃ O ₃ ⁻ (72), 235.09746 - C ₁₃ H ₁₅ O ₄ ⁻ (48), 245.08177 - C ₁₄ H ₁₃ O ₄ ⁻ (11), 246.08536 (13)	411.21698	121.06512 - C ₈ H ₉ O ⁺ (16), 123.04427 - C ₇ H ₇ O ₂ ⁺ (12), 133.02875 - C ₈ H ₅ O ₂ ⁺ (17), 133.06503 - C ₉ H ₉ O ⁺ (21), 149.02341 - C ₈ H ₅ O ₃ ⁺ (18), 149.05998 - C ₉ H ₉ O ₂ ⁺ (12), 151.03914 - C ₈ H ₇ O ₃ ⁺ (11), 157.10153 (22), 167.03436 - C ₈ H ₇ O ₄ ⁺ (19), 173.09633 - C ₁₂ H ₁₃ O ⁺ (41), 175.11197 - C ₁₂ H ₁₅ O ⁺ (100), 176.11540 (19), 185.09634 - C ₁₃ H ₁₃ O ⁺ (13), 187.11205 - C ₁₃ H ₁₅ O ⁺ (18), 189.09122 - C ₁₂ H ₁₃ O ₂ ⁺ (33), 190.09454 (39), 205.08617 - C ₁₂ H ₁₃ O ₃ ⁺ (28), 206.08932 (14), 215.10710 - C ₁₄ H ₁₅ O ₂ ⁺ (14)	Kanzonol Y or Glycybridin C
G25	C ₂₅ H ₂₆ O ₅ (0.981)	405.17090	102.94903 (19), 132.97914 (20), 146.93857 (11), 149.02443 - C ₈ H ₅ O ₃ ⁻ (10), 201.09224 - C ₁₃ H ₁₃ O ₂ ⁻ (14), 221.08177 - C ₁₂ H ₁₃ O ₄ ⁻ (38), 231.06636 - C ₁₃ H ₁₁ O ₄ ⁻ (13), 261.89008 (14), 201.09224 - C ₁₃ H ₁₃ O ₂ ⁻ (14), 221.08177 - C ₁₂ H ₁₃ O ₄ ⁻ (38), 231.06636 - C ₁₃ H ₁₁ O ₄ ⁻ (13), 261.89008 (14),	407.18570	69.07004 - C ₅ H ₉ ⁺ (6), 149.02351 - C ₈ H ₅ O ₃ ⁺ (10), 167.03407 - C ₈ H ₇ O ₄ ⁺ (97), 267.06549 - C ₁₆ H ₁₁ O ₄ ⁺ (29), 352.12619 (8)	Licocoumarin A

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound
			159.08162 - C ₁₁ H ₁₁ O [•] (14), 161.02426 - C ₉ H ₅ O ₃ [•] (24), 177.09198 - C ₁₁ H ₁₃ O ₂ [•] (100), 178.09550 (10), 189.09215 (10), 199.07661 - C ₁₃ H ₁₁ O ₂ [•] (11), 124.01651 - C ₆ H ₄ O ₃ [•] (14), 149.09706 - C ₁₀ H ₁₃ O [•] (18), 151.07635 - C ₉ H ₁₁ O ₂ [•] (14), 193.08671 - C ₁₁ H ₁₃ O ₃ [•] (100), 194.09019 (12), 229.08676 - C ₁₄ H ₁₃ O ₃ [•] (41)	293.04565 - C ₁₇ H ₉ O ₅ [•] (21), 307.06104 - C ₁₈ H ₁₁ O ₅ [•] (11), 336.10065 - C ₂₀ H ₁₆ O ₅ [•] (22), 377.17560 - C ₂₄ H ₂₅ O ₄ [•] (37), 378.17981 (12), 405.17041 - C ₂₅ H ₂₅ O ₅ [•] (15)	295.06039 - C ₁₇ H ₁₁ O ₅ ⁺ (100), 296.06345 (21), 305.11771 - C ₂₀ H ₁₇ O ₃ ⁺ (11),	
G-I-26	C ₂₅ H ₂₈ O ₆ (0.341)	423.18152		425.19601	69.07006 - C ₃ H ₉ ⁺ (11), 123.04411 - C ₇ H ₇ O ₂ ⁺ (10), 135.04414 - C ₈ H ₇ O ₂ ⁺ (34), 139.03909 - C ₇ H ₇ O ₃ ⁺ (100), 140.04243 (7), 147.04414 - C ₉ H ₇ O ₂ ⁺ (52), 165.05475 - C ₉ H ₉ O ₃ ⁺ (9), 175.03912 - C ₁₀ H ₇ O ₃ ⁺ (80), 176.04239 (10), 179.03401 (40), 191.10677 - C ₉ H ₇ O ₄ ⁺ (16), 193.04979 - C ₁₀ H ₉ O ₄ ⁺ (11), 295.06039 - C ₁₇ H ₁₁ O ₅ ⁺ (9), 313.07080 - C ₁₇ H ₁₃ O ₆ ⁺ (44), 314.07419 (9)	Gancaonin E
G27	C ₂₅ H ₃₀ O ₄ (0.365)	393.20740	102.94913 (20), 145.94185 (12), 146.93863 (31), 148.05304 - C ₉ H ₈ O ₂ [•] (16), 177.09198 - C ₁₁ H ₁₃ O ₂ [•] (44), 189.09203 - C ₁₂ H ₁₃ O ₂ [•] (23), 203.10774 - C ₁₃ H ₁₅ O ₂ [•] (100), 204.11096 (16), 215.10764 - C ₁₄ H ₁₅ O ₂ [•] (14)	395.22183	69.07005 - C ₃ H ₉ ⁺ (8), 123.04418 - C ₇ H ₇ O ₂ ⁺ (8), 135.04416 - C ₈ H ₇ O ₂ ⁺ (100), 137.05974 - C ₈ H ₉ O ₂ ⁺ (20), 147.04420 - C ₉ H ₇ O ₂ ⁺ (9), 149.05989 - C ₉ H ₉ O ₂ ⁺ (24), 161.05984 - C ₁₀ H ₉ O ₂ ⁺ (34), 189.09123 - C ₁₂ H ₁₃ O ₂ ⁺ (10), 191.10678 - C ₁₂ H ₁₅ O ₂ ⁺ (82), 192.11015 (11), 283.09674 - C ₁₇ H ₁₅ O ₄ ⁺ (5)	Kanzonol X
G28	C ₂₁ H ₂₂ O ₄ (0.013)	337.14456	79.05542 - C ₆ H ₇ [•] (9), 102.94905 (9), 107.05038 - C ₇ H ₇ O [•] (41), 108.02184 - C ₆ H ₄ O ₂ [•] (11), 123.04514 - C ₇ H ₇ O ₂ [•] (19), 134.03729 - C ₈ H ₆ O ₂ [•] (29), 149.06064 - C ₉ H ₉ O ₂ [•] (45), 175.07629 - C ₁₁ H ₁₁ O ₂ [•] (33), 187.07645 - C ₁₂ H ₁₁ O ₂ [•] (12), 201.09196 - C ₁₃ H ₁₃ O ₂ [•] (100), 202.09546 (14), 261.89026 (9), 279.06586 - C ₁₇ H ₁₁ O ₄ [•] (8)	339.15909	107.04930 - C ₇ H ₉ O ⁺ (9), 109.06496 - C ₇ H ₉ O ⁺ (12), 135.08061 - C ₉ H ₁₁ O ⁺ (11), 137.05991 - C ₈ H ₉ O ₂ ⁺ (100), 138.06322 (10), 147.04425 - C ₉ H ₇ O ₂ ⁺ (13), 147.08061 - C ₁₀ H ₁₁ O ⁺ (24), 163.07552 - C ₁₀ H ₁₁ O ₂ ⁺ (30), 173.05997 - C ₁₁ H ₉ O ₂ ⁺ (16), 189.09123 - C ₁₂ H ₁₃ O ₂ ⁺ (25)	4'-Methoxyglabridin
G29	C ₂₅ H ₂₄ O ₄ (0.885)	387.16010	n.d.	389.17508	147.08040 - C ₁₀ H ₁₁ O ⁺ (10), 189.09100 - C ₁₂ H ₁₃ O ₂ ⁺ (9), 279.06534 - C ₁₇ H ₁₁ O ₄ ⁺ (9), 291.06573 - C ₁₈ H ₁₁ O ₄ ⁺ (24), 305.11768 - C ₂₀ H ₁₇ O ₃ ⁺ (10), 318.08951 - C ₂₀ H ₁₄ O ₄ ⁺ (16), 319.09702 - C ₂₀ H ₁₅ O ₄ ⁺ (63), 333.11255 - C ₂₁ H ₁₇ O ₄ ⁺ (100), 334.11685 (32), 347.12817 - C ₂₂ H ₁₉ O ₄ ⁺ (32), 374.15289 - C ₂₄ H ₂₂ O ₄ ⁺ (13), 389.17532 - C ₂₅ H ₂₅ O ₄ ⁺ (83), 390.17825 (22)	Kanzonol E isomer
G30	C ₂₄ H ₂₈ O ₅ (0.402)	395.18649	108.02003 - C ₆ H ₄ O ₂ [•] (17), 122.03570 - C ₇ H ₆ O ₂ [•] (14), 146.93712 (12), 177.09081 - C ₁₁ H ₁₃ O ₂ [•] (100), 178.09418 (12), 189.09091 - C ₁₂ H ₁₃ O ₂ [•] (10), 217.08612 - C ₁₃ H ₁₃ O ₃ [•] (33)	397.20111	123.04444 - C ₇ H ₇ O ₂ ⁺ (26), 135.04433 - C ₈ H ₇ O ₂ ⁺ (100), 163.03917 - C ₉ H ₇ O ₃ ⁺ (21), 267.06549 - C ₁₆ H ₁₁ O ₄ ⁺ (27)	n.i. Double 3,3-DMA prenylated
G31	C ₂₅ H ₂₈ O ₄ (0.824)	n.d.	n.d.	393.20636	69.07010 - C ₃ H ₉ ⁺ (50), 123.04419 - C ₇ H ₇ O ₂ ⁺ (19), 135.04422 - C ₈ H ₇ O ₂ ⁺ (23), 147.04425 - C ₉ H ₇ O ₂ ⁺ (28), 147.08061 - C ₁₀ H ₁₁ O ⁺ (51), 149.02356 (37), 149.05998 - C ₈ H ₅ O ₃ ⁺ (35), 161.05994 - C ₁₀ H ₉ O ₂ ⁺ (12), 171.08058 - C ₁₂ H ₁₁ O ⁺ (15), 173.09647 - C ₁₂ H ₁₃ O ⁺ (17), 175.07559 - C ₁₁ H ₁₁ O ₂ ⁺ (28), 189.09123 - C ₁₂ H ₁₃ O ₂ ⁺ (100), 190.09428 (14), 191.10686 - C ₁₂ H ₁₅ O ₂ ⁺ (92),	8-Prenylphaseollinisoflavan

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound	
					150.02699 (22), 192.11017 (16)		
G32	n.i.	659.22961	n.d.	661.24365	189.09128 – C ₁₂ H ₁₃ O ₂ ⁺ (100), 190.09453 (13), 337.10745 – C ₂₀ H ₁₇ O ₅ ⁺ (16), 351.12305 – C ₂₀ H ₁₉ O ₅ ⁺ (52), 605.18085 – C ₂₉ H ₃₃ O ₁₄ ⁺ (11)	n.i. Double 3,3-DMA prenylated	
G33	C ₂₅ H ₂₈ O ₄ (0.138)	391.19168	107.05032 - C ₇ H ₇ O ⁺ (14), 146.96118 (20), 148.05310 - C ₉ H ₈ O ₂ ⁺ (12), 174.95613 (13), 175.07643 - C ₁₁ H ₁₁ O ₂ ⁺ (23), 177.09203 - C ₁₁ H ₁₃ O ₂ ⁺ (30), 187.07632 - C ₁₂ H ₁₁ O ₂ ⁺ (18),	188.11617 (20), 189.09215 - C ₁₂ H ₁₃ O ₂ ⁺ (15), 201.09204 - C ₁₃ H ₁₃ O ₂ ⁺ (100), 202.09555 (12), 203.10768 - C ₁₃ H ₁₅ O ₂ ⁺ (90), 204.11125 (13), 213.09201 - C ₁₄ H ₁₃ O ₂ ⁺ (13)	393.20609 135.04420 - C ₈ H ₇ O ₂ ⁺ (100), 147.04425 - C ₉ H ₇ O ₂ ⁺ (11), 147.08060 - C ₁₀ H ₁₁ O ⁺ (22), 161.05988 - C ₁₀ H ₉ O ₂ ⁺ (48), 173.05994 - C ₁₁ H ₉ O ₂ ⁺ (20), 189.09123 - C ₁₂ H ₁₃ O ₂ ⁺ (66), 191.10681 - C ₁₂ H ₁₅ O ₂ ⁺ (19),	Hispaglabridin A	
G35	C ₂₅ H ₂₈ O ₅ (0.683)	407.18640	148.05292 - C ₉ H ₈ O ₂ ⁺ (10), 203.10764 - C ₁₃ H ₁₅ O ₂ ⁺ (100),	409.20123 204.11084 (15), 221.08173 - C ₁₂ H ₁₃ O ₄ ⁺ (13)	167.03409 – C ₈ H ₇ O ₄ ⁺ (100), 168.03746 (8)	Glyinflanin A	
G36	C ₂₄ H ₂₄ O ₄ (-0.348)	374.15244	107.04861 – C ₇ H ₇ O ⁺ (11), 319.09723 – C ₂₀ H ₁₅ O ₄ ⁺ (100), 320.10077 (23), 331.09723 – C ₂₁ H ₁₅ O ₄ ⁺ (65), 332.10120 (18),	376.16669 359.12885 – C ₂₃ H ₁₈ O ₄ ⁺ (14), 375.15958 – C ₂₄ H ₂₃ O ₄ ⁺ (16)	69.07076 – C ₅ H ₉ ⁺ (28), 293.08093 – C ₁₈ H ₁₃ O ₄ ⁺ (59), 293.11688 – C ₁₉ H ₁₇ O ₃ ⁺ (14), 305.08102 – C ₁₉ H ₁₃ O ₄ ⁺ (90), 306.08557 (25),	n.i. Single 3,3-DMA prenylated on C3' B-ring	
G37	C ₃₀ H ₄₄ O ₄ (0.988)	467.31662	n.d.	469.33170	95.08562 – C ₇ H ₁₁ ⁺ (44), 107.08559 – C ₈ H ₁₁ ⁺ (15), 119.08575 – C ₉ H ₁₁ ⁺ (23), 121.10130 – C ₉ H ₁₃ ⁺ (29), 133.10126 – C ₁₀ H ₁₃ ⁺ (20), 135.11700 – C ₁₀ H ₁₅ ⁺ (20), 147.11702 – C ₁₁ H ₁₅ ⁺ (21), 149.09645 – C ₁₀ H ₁₃ O ⁺ (20), 173.13275 – C ₁₃ H ₁₇ ⁺ (18), 175.14841 – C ₁₃ H ₁₉ ⁺ (34),	187.14839 – C ₁₄ H ₁₉ ⁺ (18), 189.16403 – C ₁₄ H ₂₁ ⁺ (54), 205.15910 – C ₁₄ H ₂₁ O ⁺ (21), 217.15894 – C ₁₅ H ₂₁ O ⁺ (34), 233.15372 – C ₁₅ H ₂₁ O ₂ ⁺ (28), 235.16966 – C ₁₅ H ₂₃ O ₂ ⁺ (19), 317.21161 – C ₂₀ H ₂₉ O ₃ ⁺ (30), 423.32626 – C ₂₉ H ₄₃ O ₂ ⁺ (33), 469.33194 – C ₃₀ H ₄₅ O ₄ ⁺ (100)	3-Oxoglycyrhithenic acid
G38	C ₂₅ H ₂₄ O ₄ (0.848)	n.d.	n.d.	388.16724 ^(c)	173.05995 – C ₁₁ H ₉ O ₂ ⁺ (23), 333.11215 – C ₂₁ H ₁₇ O ₄ ⁺ (12), 345.11240 – C ₂₂ H ₁₇ O ₄ ⁺ (100), 346.11542 (26), 357.11212 – C ₂₃ H ₁₇ O ₄ ⁺ (14),	372.13461 – C ₂₄ H ₂₀ O ₄ ⁺ (10), 373.14365 – C ₂₄ H ₂₁ O ₄ ⁺ (86), 374.14734 (27), 387.15936 – C ₂₅ H ₂₃ O ₄ ⁺ (43), 388.16266 (23)	n.i. At least single 2,2-DMP prenylated
G39	C ₂₅ H ₂₆ O ₄ (-0.117)	389.17610	107.05036 - C ₇ H ₇ O ⁺ (7), 175.07632 - C ₁₁ H ₁₁ O ₂ ⁺ (22), 187.07645 - C ₁₂ H ₁₁ O ₂ ⁺ (12), 201.09201 - C ₁₃ H ₁₃ O ₂ ⁺ (100), 202.09540 (14)	391.19034 147.04422 - C ₉ H ₇ O ₂ ⁺ (15), 147.08058 - C ₁₀ H ₁₁ O ⁺ (47), 149.02356 - C ₈ H ₅ O ₃ ⁺ (8), 161.09595 - C ₁₀ H ₉ O ₂ ⁺ (3), 171.08061 - C ₁₂ H ₁₁ O ⁺ (12),	173.05992 - C ₁₁ H ₉ O ₂ ⁺ (14), 189.09119 - C ₁₂ H ₁₃ O ₂ ⁺ (100), 190.09453 (13), 215.10692 - C ₁₄ H ₁₅ O ₂ ⁺ (9)	Hispaglabridin B	
G40	C ₃₀ H ₄₆ O ₂ (0.894)	455.35312 ^(d)	174.95595 (9), 455.35297 - C ₃₀ H ₄₇ O ₃ ⁺ (100), 456.35641 (36)	439.35745	57.07033 - C ₄ H ₉ ⁺ (10), 67.05446 - C ₃ H ₇ ⁺ (11), 69.07010 - C ₅ H ₉ ⁺ (15), 81.07000 - C ₆ H ₉ ⁺ (70), 95.08565 - C ₇ H ₁₁ ⁺ (100),	109.10136 - C ₈ H ₁₃ ⁺ (41), 121.10135 - C ₉ H ₁₃ ⁺ (10), 123.11698 - C ₉ H ₁₅ ⁺ (43), 137.13268 - C ₁₀ H ₁₇ ⁺ (70), 213.16399 - C ₆ H ₂₁ ⁺ (13)	n.i. Not prenylated

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound	
G41	n.i.	n.d.	n.d.	n.d.	n.d.	n.i. Double chain prenylated	
<i>G. inflata</i>							
I-U-4	C ₁₅ H ₁₂ O ₅ (-0.146)	271.06131	63.02239 (23), 65.00163 (36), 83.01217 (22),	119.04865 – C ₈ H ₇ O [•] (100), 120.05200 (10), 151.00229 – C ₇ H ₅ O ₄ [•] (15)	273.07571 55.93539 (13), 91.05492 (16), 119.04954 – C ₈ H ₇ O ⁺ (32),	147.04425 – C ₉ H ₇ O ₂ ⁺ (22), 153.01843 – C ₇ H ₅ O ₄ ⁺ (100), 194.94382 (11)	Naringenin
I-U-6	C ₁₆ H ₁₄ O ₄ (0.275)	269.08182	95.01419 - C ₅ H ₃ O ₂ [•] (26), 108.02182 - C ₆ H ₄ O ₂ [•] (54), 123.04520 - C ₇ H ₇ O ₂ [•] (11), 132.02162 - C ₈ H ₄ O ₂ [•] (12),	133.02946 - C ₈ H ₅ O ₂ [•] (100), 134.03284 (10), 161.02441 - C ₉ H ₅ O ₃ [•] (31)	271.08096 65.03885 (12), 107.04926 - C ₇ H ₇ O ⁺ (18), 111.04417 - C ₆ H ₇ O ₂ ⁺ (15),	121.02855 - C ₇ H ₅ O ₂ ⁺ (100), 121.03974 (15), 134.03638 - C ₈ H ₆ O ₂ ⁺ (13)	Echinatin
I7	C ₂₀ H ₁₆ O ₆ (-0.084)	351.08759	65.00166 (39), 83.01215 (51), 102.94711 (20), 107.01225 (13), 107.04855 (10), 151.00233 – C ₇ H ₅ O ₄ [•] (24), 175.03867 – C ₁₀ H ₇ O ₃ [•] (15), 199.07542 – C ₁₃ H ₁₁ O ₂ [•] (100), 200.07899 (11),	223.07545 – C ₁₅ H ₁₁ O ₂ [•] (13), 239.10739 – C ₁₆ H ₁₅ O ₂ [•] (13), 241.08653 – C ₁₅ H ₁₃ O ₃ [•] (52), 265.08682 – C ₁₇ H ₁₃ O ₃ [•] (35), 267.06586 – C ₁₆ H ₁₁ O ₄ [•] (17), 283.09738 – C ₁₇ H ₁₅ O ₄ [•] (65), 284.10049 (13), 321.04031 – C ₁₈ H ₉ O ₆ [•] (14), 335.05521 – C ₁₉ H ₁₁ O ₆ [•] (14)	353.10193 81.07067 – C ₆ H ₉ ⁺ (28), 109.06532 – C ₇ H ₉ O ⁺ (25), 153.01843 – C ₇ H ₅ O ₄ ⁺ (85), 217.04988 – C ₁₂ H ₉ O ₄ ⁺ (26), 218.86853 (10), 255.06551 – C ₁₅ H ₁₁ O ₄ ⁺ (37), 260.93335 (16), 261.90201 (16),	271.06021 – C ₁₅ H ₁₁ O ₅ ⁺ (10), 283.06039 – C ₁₆ H ₁₁ O ₅ ⁺ (51), 299.05530 – C ₁₆ H ₁₁ O ₆ ⁺ (42), 307.09653 – C ₁₉ H ₁₅ O ₄ ⁺ (14), 311.05527 – C ₁₇ H ₁₁ O ₆ ⁺ (100), 312.05741 (22), 335.09180 – C ₂₀ H ₁₅ O ₅ ⁺ (15), 353.10236 – C ₂₀ H ₁₇ O ₆ ⁺ (16)	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B
I-U-8	C ₂₀ H ₁₈ O ₆ (0.099)	353.10327	57.03299 (24), 83.01219 (13), 102.94712 (13), 125.02287 – C ₆ H ₅ O ₃ [•] (100),	181.89633 (19), 183.91205 (24), 227.07068 – C ₁₄ H ₁₁ O ₃ [•] (19)	355.11765 123.04443 – C ₇ H ₇ O ₂ ⁺ (44), 127.03931 – C ₆ H ₇ O ₃ ⁺ (12), 147.04422 – C ₉ H ₇ O ₂ ⁺ (10), 147.08067 – C ₁₀ H ₁₁ O ⁺ (11), 151.03923 – C ₈ H ₇ O ₃ ⁺ (81),	153.01846 – C ₇ H ₅ O ₄ ⁺ (11), 179.03415 – C ₉ H ₇ O ₄ ⁺ (100), 189.09128 – C ₁₂ H ₁₃ O ₂ ⁺ (16), 201.09132 – C ₁₃ H ₁₃ O ₂ ⁺ (38), 218.86864 (28)	Licoisoflavanone
I10	C ₂₀ H ₂₀ O ₆ (-0.322)	355.11896	57.03299 (23), 83.01218 (12), 125.02287 – C ₆ H ₅ O ₃ [•] (100), 229.08630 – C ₁₄ H ₁₃ O ₃ [•] (17)		357.13315 123.04439 – C ₇ H ₇ O ₂ ⁺ (10), 127.03934 – C ₆ H ₇ O ₃ ⁺ (10), 137.02361 – C ₇ H ₅ O ₃ ⁺ (11), 147.04430 – C ₇ H ₇ O ₂ ⁺ (100),	175.03929 – C ₁₀ H ₇ O ₃ ⁺ (81), 179.03426 – C ₉ H ₇ O ₄ ⁺ (13), 270.08447 (12), 283.06055 – C ₁₆ H ₁₁ O ₅ ⁺ (18)	n.i. A-ring 3,3-DMA prenylated without <i>ortho</i> -OCH ₃
I-U-12	C ₂₀ H ₁₆ O ₆ (-0.268)	351.08765	102.94719 (14), 107.01231 – C ₆ H ₅ O ₂ [•] (16), 125.02299 – C ₆ H ₅ O ₃ [•] (15), 151.00230 – C ₇ H ₅ O ₄ [•] (30), 177.01797 – C ₉ H ₅ O ₄ [•] (35), 199.07578 – C ₁₃ H ₁₁ O ₂ [•] (14), 203.03389 – C ₁₁ H ₇ O ₄ [•] (31), 284.03168 – C ₁₅ H ₈ O ₆ [•] (11), 293.04578 – C ₁₇ H ₉ O ₅ [•] (14), 307.06122 – C ₁₈ H ₁₁ O ₅ [•] (13),	321.04053 – C ₁₈ H ₉ O ₆ [•] (81), 322.04440 (19), 323.09265 – C ₁₉ H ₁₅ O ₅ [•] (33), 324.09613 (12), 333.07690 – C ₂₀ H ₁₃ O ₅ [•] (61), 334.07974 (23), 335.05536 – C ₁₉ H ₁₁ O ₆ [•] (33), 336.06317 (29), 351.08752 – C ₂₀ H ₁₅ O ₆ [•] (100), 352.09076 (19)	353.10187 153.01839 – C ₇ H ₅ O ₄ ⁺ (100), 311.05515 – C ₁₇ H ₁₁ O ₆ ⁺ (15)	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B	
I13	C ₂₀ H ₁₈ O ₅ (-0.059)	337.10840	91.01725 (17), 102.94718 (16), 117.03296 (37), 133.06445 – C ₉ H ₉ O [•] (10), 135.00716 – C ₇ H ₇ O ₃ [•] (16), 153.01788 – C ₇ H ₅ O ₄ [•] (35), 161.02330 – C ₉ H ₅ O ₃ [•] (10),	240.04237 – C ₁₄ H ₈ O ₄ [•] (14), 243.87941 (28), 261.89023 (42), 267.02966 – C ₁₅ H ₇ O ₅ [•] (14), 268.03751 – C ₁₅ H ₈ O ₅ [•] (100), 269.04080 (15), 281.04547 – C ₁₆ H ₉ O ₅ [•] (12),	339.12268 201.05487 – C ₁₂ H ₉ O ₃ ⁺ (12), 283.06030 – C ₁₆ H ₁₁ O ₅ ⁺ (100), 284.06366 (20)	Licoflavone C	

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound	
I-U-14	C ₂₁ H ₂₄ O ₅ (-0.253)	355.15533	198.03149 – C ₁₂ H ₆ O ₃ ⁻ (12), 211.03923 – C ₁₃ H ₇ O ₃ ⁻ (11), 224.04721 – C ₁₄ H ₈ O ₃ ⁻ (38),	357.16956	65.03956 (10), 123.04449 – C ₇ H ₇ O ₂ ⁺ (100), 135.04437 – C ₈ H ₇ O ₂ ⁺ (10), 137.06003 – C ₈ H ₉ O ₂ ⁺ (15), 165.05495 – C ₉ H ₉ O ₃ ⁺ (32)	Glyasperin C	
			91.05362 (17), 109.02786 – C ₆ H ₅ O ₂ ⁻ (44), 121.02789 – C ₇ H ₅ O ₂ ⁻ (22), 124.01488 – C ₆ H ₄ O ₃ ⁻ (20), 135.04362 – C ₈ H ₇ O ₂ ⁻ (100), 137.02272 – C ₇ H ₅ O ₃ ⁻ (19), 147.04361 – C ₉ H ₇ O ₂ ⁻ (17), 149.02298 – C ₈ H ₅ O ₃ ⁻ (20), 151.03897 – C ₈ H ₇ O ₃ ⁻ (17), 163.03867 – C ₉ H ₇ O ₃ ⁻ (27),				175.03856 – C ₁₀ H ₇ O ₃ ⁻ (14), 181.89621 (41), 183.91194 (45), 191.07022 – C ₁₁ H ₁₁ O ₃ ⁻ (17), 203.07037 – C ₁₂ H ₁₁ O ₃ ⁻ (23), 203.10698 – C ₁₃ H ₁₅ O ₂ ⁻ (20), 207.10172 – C ₁₂ H ₁₅ O ₃ ⁻ (14), 218.09401 – C ₁₃ H ₁₄ O ₃ ⁻ (16), 231.10173 – C ₁₄ H ₁₅ O ₃ ⁻ (14), 233.11737 – C ₁₄ H ₁₇ O ₃ ⁻ (18)
I-U-15	C ₂₀ H ₁₈ O ₆ (0.099)	353.10312	57.03298 (18), 125.02285 – C ₆ H ₅ O ₃ ⁻ (100), 183.91199 (11)	355.11765	123.04441 – C ₇ H ₇ O ₂ ⁺ (39), 127.03927 – C ₆ H ₇ O ₃ ⁺ (11), 147.08067 – C ₁₀ H ₁₁ O ⁺ (12), 151.03922 – C ₈ H ₇ O ₃ ⁺ (79), 153.01845 – C ₇ H ₅ O ₄ ⁺ (11), 179.03409 – C ₉ H ₇ O ₄ ⁺ (100), 180.03734 (10), 187.07568 – C ₁₂ H ₁₁ O ₂ ⁺ (10), 189.09119 – C ₁₂ H ₁₃ O ₂ ⁺ (20), 201.09131 – C ₁₂ H ₁₃ O ₂ ⁺ (37), 337.10718 – C ₂₀ H ₁₇ O ₅ ⁺ (11)	Uralenin	
I-U-16	C ₂₀ H ₁₈ O ₆ (0.099)	353.10303	65.00162 (43), 83.01213 (44), 125.02277 – C ₆ H ₅ O ₃ ⁻ (16), 151.00232 – C ₇ H ₃ O ₄ ⁻ (17), 174.03087 – C ₁₀ H ₆ O ₃ ⁻ (13), 201.09103 – C ₁₃ H ₁₃ O ₂ ⁻ (87), 202.09471 (14), 211.03923 – C ₁₃ H ₇ O ₃ ⁻ (17), 212.04747 – C ₁₃ H ₈ O ₃ ⁻ (17), 214.02623 – C ₁₂ H ₆ O ₄ ⁻ (35),	216.04196 – C ₁₂ H ₈ O ₄ ⁻ (58), 240.04192 – C ₁₄ H ₈ O ₄ ⁻ (14), 243.10216 – C ₁₅ H ₁₅ O ₃ ⁻ (60), 267.10214 – C ₁₇ H ₁₅ O ₃ ⁻ (26), 269.08151 – C ₁₆ H ₁₃ O ₄ ⁻ (14), 283.02414 – C ₁₅ H ₇ O ₆ ⁻ (17), 284.03229 – C ₁₈ H ₈ O ₆ ⁻ (100), 285.03564 (17), 285.11295 – C ₁₇ H ₁₇ O ₄ ⁻ (44), 353.10303 – C ₂₀ H ₁₇ O ₆ ⁻ (13)	355.11765	147.04425 – C ₉ H ₇ O ₂ ⁺ (15), 153.01840 – C ₇ H ₅ O ₄ ⁺ (12), 217.04977 – C ₁₂ H ₉ O ₄ ⁺ (19), 243.06534 – C ₁₄ H ₁₁ O ₄ ⁺ (15), 271.06027 – C ₁₅ H ₁₁ O ₅ ⁺ (11), 299.05521 – C ₁₆ H ₁₁ O ₆ ⁺ (100), 300.05872 (20)	Licoisoflavone A
I17	C ₂₁ H ₂₂ O ₄ (0.720)	337.14459	93.03291 – C ₆ H ₅ O ⁻ (100), 108.02006 – C ₆ H ₄ O ₂ ⁻ (31), 161.05943 – C ₁₀ H ₉ O ₂ ⁻ (34), 187.03905 – C ₁₁ H ₇ O ₃ ⁻ (13), 187.07530 – C ₁₂ H ₁₁ O ₂ ⁻ (41),	201.09102 – C ₁₃ H ₁₃ O ₂ ⁻ (33), 229.08629 – C ₁₄ H ₁₃ O ₃ ⁻ (26), 281.08167 – C ₁₇ H ₁₃ O ₄ ⁻ (16), 305.11786 – C ₂₀ H ₁₇ O ₃ ⁻ (10), 307.09747 – C ₁₉ H ₁₅ O ₄ ⁻ (13)	339.15933	121.02890 – C ₇ H ₅ O ₂ ⁺ (100)	Licochalcone A
I-U-18	C ₂₀ H ₁₈ O ₅ (-0.059)	337.10846	93.03291 – C ₆ H ₅ O ⁻ (32), 102.94706 (15), 199.07549 – C ₁₃ H ₁₁ O ₂ ⁻ (13), 201.09113 – C ₁₃ H ₁₃ O ₂ ⁻ (13), 243.87950 (24), 261.89014 (33),	267.02963 – C ₁₅ H ₇ O ₅ ⁻ (30), 281.04520 – C ₁₆ H ₉ O ₅ ⁻ (100), 282.04916 (23), 293.04507 – C ₁₇ H ₉ O ₅ ⁻ (32), 337.10803 – C ₂₀ H ₁₇ O ₅ ⁻ (64), 338.11121 (15)	339.12268	69.07076 – C ₅ H ₉ ⁺ (100), 121.02876 – C ₇ H ₅ O ₂ ⁺ (40), 153.01849 – C ₇ H ₅ O ₄ ⁺ (15), 255.06531 – C ₁₅ H ₁₁ O ₄ ⁺ (32), 271.06024 – C ₁₅ H ₁₁ O ₅ ⁺ (62), 283.06021 – C ₁₆ H ₁₁ O ₅ ⁺ (39)	3'-Prenylgenistein (Isowighteone)
I-U-19	C ₂₁ H ₁₈ O ₆ (0.096)	365.10287	294.01694 – C ₁₆ H ₆ O ₆ ⁻ (18), 295.02435 – C ₁₆ H ₇ O ₆ ⁻ (42), 306.01685 – C ₁₇ H ₆ O ₆ ⁻ (25), 307.02448 – C ₁₇ H ₇ O ₆ ⁻ (100), 308.02798 (22)	367.11765	253.04985 – C ₁₈ H ₉ O ₄ ⁺ (36), 255.06551 – C ₁₅ H ₁₁ O ₄ ⁺ (12), 268.03720 – C ₁₅ H ₈ O ₅ ⁺ (15), 272.03189 – C ₁₄ H ₈ O ₆ ⁺ (10), 275.89056 (12), 283.06036 – C ₁₆ H ₁₁ O ₅ ⁺ (31), 296.03183 – C ₁₆ H ₈ O ₆ ⁺ (100), 297.03796 – C ₁₆ H ₉ O ₆ ⁺ (41), 309.03955 – C ₁₇ H ₉ O ₆ ⁺ (26), 311.05518 – C ₁₇ H ₁₁ O ₆ ⁺ (71),	Glycyrol	

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound	
I-U-20	C ₂₀ H ₁₆ O ₆ (-0.353)	351.08734	65.00164 (27), 83.01218 (35), 151.00217 – C ₇ H ₃ O ₄ ⁻ (12), 175.03894 – C ₁₀ H ₇ O ₃ ⁻ (11), 199.07547 – C ₁₃ H ₁₁ O ₂ ⁻ (55), 239.10712 – C ₁₆ H ₁₅ O ₂ ⁻ (13), 241.08659 – C ₁₅ H ₁₃ O ₃ ⁻ (46), 242.09019 (11),	353.10184	281.04471 – C ₁₆ H ₉ O ₅ ⁺ (73), 282.04828 (16), 81.07069 – C ₆ H ₉ ⁺ (32), 109.06528 – C ₇ H ₉ O ⁺ (26), 153.01843 – C ₇ H ₅ O ₄ ⁺ (92), 191.03415 – C ₁₀ H ₇ O ₄ ⁺ (13), 217.04987 – C ₁₂ H ₉ O ₄ ⁺ (27), 255.06532 – C ₁₅ H ₁₁ O ₄ ⁺ (36), 271.06021 – C ₁₅ H ₁₁ O ₅ ⁺ (12), 283.06033 – C ₁₆ H ₁₁ O ₅ ⁺ (53),	312.05872 (15)	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B
					299.05518 – C ₁₆ H ₁₁ O ₆ ⁺ (54), 300.05841 (12), 307.09677 – C ₁₉ H ₁₅ O ₄ ⁺ (12), 311.05524 – C ₁₇ H ₁₁ O ₆ ⁺ (100), 312.05853 (21), 335.09131 – C ₂₀ H ₁₅ O ₅ ⁺ (16), 353.10245 – C ₂₀ H ₁₇ O ₆ ⁺ (24)		
I22	C ₂₀ H ₁₆ O ₅ (-0.356)	335.09274	151.00215 – C ₇ H ₃ O ₄ ⁻ (17), 176.01027 – C ₉ H ₄ O ₄ ⁻ (13), 243.87939 (17), 261.89023 (29), 291.06644 – C ₁₈ H ₁₁ O ₄ ⁻ (13), 305.04529 – C ₁₈ H ₉ O ₅ ⁻ (92),	337.10693	153.01843 – C ₇ H ₅ O ₄ ⁺ (100), 295.06039 – C ₁₇ H ₁₁ O ₅ ⁺ (27), 321.07599 – C ₁₉ H ₁₃ O ₅ ⁺ (12)		Isoderrone
I-U-24	C ₂₂ H ₂₆ O ₅ (-0.001)	369.17081	91.05362 (16), 109.02785 – C ₆ H ₅ O ₂ ⁻ (41), 135.04361 – C ₈ H ₇ O ₂ ⁻ (100), 147.04369 – C ₉ H ₇ O ₂ ⁻ (11),	371.18530	69.07076 – C ₅ H ₉ ⁺ (87), 123.04441 – C ₇ H ₇ O ₂ ⁺ (100), 137.05998 – C ₈ H ₉ O ₂ ⁺ (12), 149.05992 – C ₉ H ₉ O ₂ ⁺ (23),	167.07050 – C ₉ H ₁₁ O ₃ ⁺ (98), 179.07054 – C ₁₀ H ₁₁ O ₃ ⁺ (15), 181.08614 – C ₁₀ H ₁₃ O ₃ ⁺ (27), 193.08630 – C ₁₁ H ₁₃ O ₃ ⁺ (15)	Glyasperin D
I25	C ₂₅ H ₂₈ O ₅ (0.170)	407.18646	106.04078 – C ₇ H ₆ O ⁻ (16), 161.09584 – C ₁₁ H ₁₃ O ⁻ (100), 162.09917 (13), 177.09088 – C ₁₁ H ₁₃ O ₂ ⁻ (31), 185.09599 – C ₁₃ H ₁₃ O ⁻ (30),	409.20102	133.02866 – C ₈ H ₅ O ₂ ⁺ (39), 149.02356 – C ₈ H ₅ O ₃ ⁺ (36), 167.03410 – C ₈ H ₇ O ₄ ⁺ (14), 189.09125 – C ₁₂ H ₁₃ O ₂ ⁺ (100), 205.08618 – C ₁₂ H ₁₃ O ₃ ⁺ (69)		Macarangaflavanone B (Paratocarpin L)
I27	C ₂₅ H ₂₈ O ₅ (-0.050)	407.18646	132.05649 – C ₉ H ₈ O ⁻ (10), 133.06435 – C ₉ H ₉ O ⁻ (28), 151.07504 – C ₉ H ₁₁ O ₂ ⁻ (12), 175.07520 – C ₁₁ H ₁₁ O ₂ ⁻ (16),	409.20093	165.01848 – C ₈ H ₅ O ₄ ⁺ (100), 183.02905 – C ₈ H ₇ O ₅ ⁺ (67)		n.i. Double 3,3-DMA and 2,2-DMP prenylated
I28	C ₂₅ H ₂₆ O ₆ (0.130)	421.16589	133.06433 – C ₉ H ₉ O ⁻ (27), 151.07506 – C ₉ H ₁₁ O ₂ ⁻ (76), 183.91226 (29), 201.09096 – C ₁₃ H ₁₃ O ₂ ⁻ (25), 218.05820 – C ₁₂ H ₁₀ O ₄ ⁻ (18), 243.10207 – C ₁₅ H ₁₅ O ₃ ⁻ (40), 267.10217 – C ₁₇ H ₁₅ O ₃ ⁻ (25), 269.08167 – C ₁₆ H ₁₃ O ₄ ⁻ (22), 284.10501 – C ₁₇ H ₁₆ O ₄ ⁻ (25), 297.04004 – C ₁₆ H ₉ O ₆ ⁻ (34),	423.18027	219.06537 – C ₁₂ H ₁₁ O ₄ ⁺ (15), 311.05508 – C ₁₇ H ₁₁ O ₆ ⁺ (100), 312.05844 (19), 367.11780 – C ₂₁ H ₁₉ O ₆ ⁺ (26)		n.i. Double 3,3-DMA prenylated
I29	C ₂₅ H ₂₈ O ₆ (0.129)	423.18158	149.09576 – C ₁₀ H ₁₃ O ⁻ (15), 193.08597 – C ₁₁ H ₁₃ O ₃ ⁻ (100),	425.19592	135.04431 – C ₈ H ₇ O ₂ ⁺ (46), 139.03922 – C ₇ H ₇ O ₃ ⁺ (11), 191.10689 – C ₁₂ H ₁₅ O ₂ ⁺ (100),	192.11023 (13), 295.06046 – C ₁₇ H ₁₁ O ₅ ⁺ (13)	Gancaonin E isomer
I-U-30	C ₂₅ H ₂₆ O ₆ (-0.012)	421.16583	309.04019 – C ₁₇ H ₉ O ₆ ⁻ (46), 352.09494 – C ₂₀ H ₁₆ O ₆ ⁻ (28), 365.10266 – C ₂₁ H ₁₇ O ₆ ⁻ (36),	423.18021	299.05521 – C ₁₆ H ₁₁ O ₆ ⁺ (40), 311.05521 – C ₁₇ H ₁₁ O ₆ ⁺ (100), 312.05859 (19),	368.12143 (22)	2'-Hydroxy-isolupalbingenin (Iso)angustone A)

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	Tentatively identified compound
			366.10916 (27), 422.16879 (31)		367.11795 – C ₂₁ H ₁₉ O ₆ ⁺ (94),	
I31	C ₂₅ H ₂₆ O ₅ (0.073)	405.17096	n.d.	407.18533	n.d.	n.i. Double 3,3-DMA prenylated
I32	C ₂₅ H ₂₆ O ₄ (0.190)	389.17609	159.08017 – C ₁₁ H ₁₁ O [•] (10), 185.09602 – C ₁₃ H ₁₃ O [•] (100), 186.09935 (15),	203.07045 – C ₁₂ H ₁₁ O ₃ [•] (11), 221.08119 – C ₁₂ H ₁₃ O ₄ [•] (24)	391.19046 149.02351 – C ₅ H ₅ O ₃ ⁺ (34), 167.03406 – C ₈ H ₇ O ₄ ⁺ (100)	Euchrenone A5
I33	C ₂₅ H ₂₆ O ₆ (0.272)	421.16589	149.09573 – C ₁₀ H ₁₃ O [•] (13), 193.08589 – C ₁₁ H ₁₃ O ₃ [•] (100),	194.08922 (11)	423.18033 189.09126 – C ₁₂ H ₁₃ O ₂ ⁺ (100), 190.09460 (13), 191.03412 – C ₁₀ H ₇ O ₄ ⁺ (27), 349.10736 – C ₂₁ H ₁₇ O ₅ ⁺ (18)	Glyurallin B
I-U-34	C ₂₅ H ₂₆ O ₅ (-0.001)	405.17087	295.06097 – C ₁₇ H ₁₁ O ₅ [•] (13), 307.06100 – C ₁₈ H ₁₁ O ₅ [•] (78), 308.06445 (16), 347.09189 – C ₂₁ H ₁₅ O ₅ [•] (11), 350.11432 – C ₂₁ H ₁₈ O ₅ [•] (10),	361.10745 – C ₂₂ H ₁₇ O ₅ [•] (16), 382.10571 (21), 405.17047 – C ₂₅ H ₂₅ O ₅ [•] (100), 406.17398 (35)	407.18530 295.06042 – C ₁₇ H ₁₁ O ₅ ⁺ (100), 296.06375 (19)	6,8-Diprenylgenistein
I35	C ₂₅ H ₂₆ O ₆ (0.059)	421.16595	109.06422 – C ₇ H ₉ O [•] (11), 133.06438 – C ₉ H ₉ O [•] (31), 151.07509 – C ₉ H ₁₁ O ₂ [•] (42), 175.07521 – C ₁₁ H ₁₁ O ₂ [•] (18), 176.01035 – C ₉ H ₄ O ₄ [•] (16), 201.09106 – C ₁₃ H ₁₃ O ₂ [•] (29), 218.05797 – C ₁₂ H ₁₀ O ₄ [•] (12), 219.06551 – C ₁₂ H ₁₁ O ₄ [•] (100), 220.06902 (13), 243.10234 – C ₁₅ H ₁₅ O ₃ [•] (21),	267.10239 – C ₁₇ H ₁₅ O ₃ [•] (15), 269.08191 – C ₁₆ H ₁₃ O ₄ [•] (15), 308.10532 – C ₁₉ H ₁₆ O ₄ [•] (11), 309.04041 – C ₁₇ H ₆ O ₆ [•] (34), 323.05557 – C ₁₈ H ₁₁ O ₆ [•] (12), 352.09515 – C ₂₀ H ₁₆ O ₆ [•] (44), 353.17578 – C ₂₂ H ₂₅ O ₄ [•] (14), 365.10324 – C ₂₁ H ₁₇ O ₆ [•] (11), 421.16556 – C ₂₅ H ₂₅ O ₆ [•] (69), 422.16904 (20)	423.18024 311.05515 – C ₁₇ H ₁₁ O ₆ ⁺ (100), 312.05862 (19)	2'-Hydroxy- isolupalbingenin ((Iso)angustone A)
I36	C ₂₅ H ₂₄ O ₆ (0.249)	419.15012	133.06439 – C ₉ H ₉ O [•] (12), 151.07503 – C ₉ H ₁₁ O ₂ [•] (26), 199.07544 – C ₁₃ H ₁₁ O ₂ [•] (30), 219.06552 – C ₁₂ H ₁₁ O ₄ [•] (55), 241.08643 – C ₁₅ H ₁₃ O ₃ [•] (13),	265.08664 – C ₁₇ H ₁₃ O ₃ [•] (14), 267.06613 – C ₁₆ H ₁₁ O ₄ [•] (11), 351.15985 – C ₂₂ H ₂₃ O ₄ [•] (13), 419.14978 – C ₂₅ H ₂₃ O ₆ [•] (100), 420.15338 (28)	421.16467 165.01854 – C ₈ H ₅ O ₄ ⁺ (100), 183.02913 – C ₈ H ₇ O ₃ ⁺ (54), 201.09134 – C ₁₃ H ₁₃ O ₂ ⁺ (17), 347.09189 – C ₂₁ H ₁₅ O ₅ ⁺ (16), 365.10248 – C ₂₁ H ₁₇ O ₆ ⁺ (92), 366.10583 (24)	Angustone B
<i>G. uralensis</i>						
U5	C ₂₁ H ₂₂ O ₆ (0.202)	369.13443	124.01502 – C ₆ H ₄ O ₃ [•] (64), 139.03857 – C ₇ H ₇ O ₃ [•] (100), 174.03099 – C ₁₀ H ₆ O ₃ [•] (16),	206.02115 – C ₁₀ H ₆ O ₅ [•] (14), 229.08636 – C ₁₄ H ₁₃ O ₃ [•] (30)	371.14899 141.05486 – C ₇ H ₉ O ₃ ⁺ (10), 147.04427 – C ₉ H ₇ O ₂ ⁺ (100), 175.03925 – C ₁₀ H ₇ O ₃ ⁺ (45)	Glyasperin B
U7	C ₂₁ H ₂₂ O ₅ (-0.113)	353.10333	102.94718 (62), 103.91856 (28), 121.02793 – C ₇ H ₅ O ₂ [•] (20), 170.03635 – C ₁₁ H ₆ O ₂ [•] (15), 173.02316 – C ₁₀ H ₅ O ₃ [•] (38), 177.09087 – C ₁₁ H ₁₃ O ₂ [•] (44), 181.89636 (100), 183.91203 (97), 201.92274 (337), 214.02632 – C ₁₂ H ₆ O ₄ [•] (42),	226.02673 – C ₁₃ H ₆ O ₄ [•] (15), 239.03445 – C ₁₄ H ₇ O ₄ [•] (16), 242.02159 – C ₁₃ H ₆ O ₅ [•] (34), 246.01657 – C ₁₂ H ₆ O ₆ [•] (22), 251.03429 – C ₁₅ H ₇ O ₄ [•] (42), 255.02971 – C ₁₄ H ₇ O ₅ [•] (27), 267.06598 – C ₁₆ H ₁₁ O ₄ [•] (44), 283.06110 – C ₁₆ H ₁₁ O ₅ [•] (17), 295.06097 – C ₁₇ H ₁₁ O ₅ [•] (70), 309.07727 – C ₁₈ H ₁₃ O ₅ [•] (16)	355.15396 123.04440 – C ₇ H ₇ O ₂ ⁺ (100),	n.i. O-3,3-DMA prenylated
U9	C ₂₁ H ₂₀ O ₆ (0.095)	367.11844	297.04016 – C ₁₆ H ₉ O ₆ [•] (29), 309.04028 – C ₁₇ H ₉ O ₆ [•] (100),		369.13330 69.07076 – C ₅ H ₉ ⁺ (16), 123.04444 – C ₇ H ₇ O ₂ ⁺ (46), 229.08601 – C ₁₄ H ₁₃ O ₃ ⁺ (23), 243.06555 – C ₁₄ H ₁₁ O ₄ ⁺ (55),	Glycycoumarin

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound
			310.04360 (18)		135.04424 – C ₈ H ₇ O ₂ ⁺ (15), 149.02353 – C ₈ H ₅ O ₃ ⁺ (21), 205.04982 – C ₁₁ H ₉ O ₄ ⁺ (20), 209.06004 – C ₁₄ H ₉ O ₂ ⁺ (15), 213.05478 – C ₁₃ H ₉ O ₃ ⁺ (23), 215.07060 – C ₁₃ H ₁₁ O ₃ ⁺ (23), 225.05479 – C ₁₄ H ₉ O ₃ ⁺ (18), 227.07043 – C ₁₄ H ₁₁ O ₃ ⁺ (21), 255.06548 – C ₁₅ H ₁₁ O ₄ ⁺ (29), 257.08105 (24), 270.05243 – C ₁₅ H ₁₀ O ₅ ⁺ (71), 271.05975 – C ₁₅ H ₁₁ O ₅ ⁺ (26), 285.07596 – C ₁₆ H ₁₃ O ₅ ⁺ (100), 286.07935 (19), 298.04858 – C ₁₆ H ₁₀ O ₆ ⁺ (37), 313.07077 – C ₁₇ H ₁₃ O ₆ ⁺ (49)	
U10	C ₂₀ H ₁₈ O ₆ (0.353)	353.10315	102.94716 (15), 151.00223 – C ₇ H ₃ O ₄ ⁻ (21), 162.03098 – C ₉ H ₆ O ₃ ⁻ (12), 181.89632 (18), 183.91205 (27), 227.03430 – C ₁₃ H ₇ O ₄ ⁻ (16), 241.05014 – C ₁₇ H ₉ O ₄ ⁻ (15), 254.05835 – C ₁₅ H ₁₀ O ₄ ⁻ (10), 255.02937 – C ₁₄ H ₇ O ₅ ⁻ (15), 269.04544 – C ₁₅ H ₉ O ₅ ⁻ (35), 283.02502 – C ₁₅ H ₇ O ₆ ⁻ (10), 284.03241 – C ₁₅ H ₈ O ₆ ⁻ (56), 297.04016 – C ₁₆ H ₉ O ₆ ⁻ (100), 298.04764 – C ₁₆ H ₁₀ O ₆ ⁻ (84), 299.05133 (12), 309.04028 – C ₁₇ H ₉ O ₆ ⁻ (13), 310.04709 (10), 353.10284 – C ₂₀ H ₁₇ O ₆ ⁻ (64), 354.10638 (15)	355.11774	69.07077 – C ₅ H ₉ ⁺ (100), 153.01837 – C ₇ H ₅ O ₄ ⁺ (15), 241.04977 (12), 243.06554 – C ₁₄ H ₁₁ O ₄ ⁺ (28), 271.06030 – C ₁₅ H ₁₁ O ₅ ⁺ (15), 287.05524 – C ₁₅ H ₁₁ O ₆ ⁺ (65), 299.05521 – C ₁₆ H ₁₁ O ₆ ⁺ (17)	Glycyrrhisoflavone
U11	C ₂₁ H ₂₂ O ₅ (-0.113)	353.10330	102.94718 (62), 103.91856 (28), 121.02793 – C ₇ H ₅ O ₂ ⁻ (20), 170.03635 – C ₁₁ H ₆ O ₂ ⁻ (15), 173.02316 – C ₁₀ H ₅ O ₃ ⁻ (38), 177.09087 – C ₁₁ H ₁₃ O ₂ ⁻ (43), 181.89636 (100), 183.91203 (97), 201.92274 (37), 214.02632 – C ₁₂ H ₆ O ₄ ⁻ (42), 149.05936 – C ₉ H ₉ O ₂ ⁻ (14), 201.01831 – C ₁₁ H ₅ O ₄ ⁻ (26), 297.03992 – C ₁₆ H ₉ O ₆ ⁻ (12), 307.09717 – C ₁₉ H ₁₅ O ₄ ⁻ (28), 308.03259 – C ₁₇ H ₈ O ₆ ⁻ (28), 311.05600 – C ₁₇ H ₁₁ O ₆ ⁻ (20), 226.02673 – C ₁₃ H ₆ O ₄ ⁻ (15), 239.03445 – C ₁₄ H ₇ O ₄ ⁻ (16), 242.02159 – C ₁₃ H ₆ O ₅ ⁻ (34), 246.01657 – C ₁₂ H ₆ O ₆ ⁻ (22), 251.03429 – C ₁₅ H ₇ O ₄ ⁻ (42), 255.02971 – C ₁₄ H ₇ O ₅ ⁻ (27), 267.06598 – C ₁₆ H ₁₁ O ₄ ⁻ (44), 283.06110 – C ₁₆ H ₁₁ O ₅ ⁻ (17), 295.06097 – C ₁₇ H ₁₁ O ₅ ⁻ (70), 309.07727 – C ₁₈ H ₁₃ O ₅ ⁻ (16)	355.15396	123.04440 – C ₇ H ₇ O ₂ ⁺ (100)	n.i. C ₆ 3,3-DMA prenylated without <i>ortho</i> -OCH ₃
U13	C ₂₂ H ₂₂ O ₆ (-0.300)	381.13443	149.05936 – C ₉ H ₉ O ₂ ⁻ (14), 201.01831 – C ₁₁ H ₅ O ₄ ⁻ (26), 297.03992 – C ₁₆ H ₉ O ₆ ⁻ (12), 307.09717 – C ₁₉ H ₁₅ O ₄ ⁻ (28), 308.03259 – C ₁₇ H ₈ O ₆ ⁻ (28), 311.05600 – C ₁₇ H ₁₁ O ₆ ⁻ (20), 323.05591 – C ₁₈ H ₁₁ O ₆ ⁻ (78), 323.09216 – C ₁₉ H ₁₅ O ₅ ⁻ (80), 324.05927 (16), 324.09506 (16), 351.08710 – C ₂₀ H ₁₅ O ₆ ⁻ (100)	383.14880	137.02359 – C ₇ H ₅ O ₃ ⁺ (29), 149.02362 – C ₈ H ₅ O ₃ ⁺ (16), 163.03922 – C ₉ H ₇ O ₃ ⁺ (22), 177.05504 – C ₁₀ H ₉ O ₃ ⁺ (22), 178.06288 – C ₁₀ H ₁₀ O ₃ ⁺ (87), 191.07065 – C ₁₁ H ₉ O ₃ ⁺ (70), 239.07065 – C ₁₅ H ₁₁ O ₃ ⁺ (16), 257.08124 – C ₁₅ H ₁₃ O ₄ ⁺ (21), 267.06580 – C ₁₆ H ₁₁ O ₄ ⁺ (22), 269.04443 – C ₁₅ H ₉ O ₅ ⁺ (17), 283.06018 – C ₁₆ H ₁₁ O ₅ ⁺ (20), 284.06830 – C ₁₆ H ₁₂ O ₅ ⁺ (32), 295.06046 – C ₁₇ H ₁₁ O ₅ ⁺ (23), 297.03989 – C ₁₆ H ₉ O ₆ ⁺ (28), 299.09189 – C ₁₇ H ₁₅ O ₅ ⁺ (100), 300.09528 (19), 311.05551 – C ₁₇ H ₁₁ O ₆ ⁺ (20), 312.06302 – C ₁₇ H ₁₂ O ₆ ⁺ (52), 327.08670 – C ₁₈ H ₁₅ O ₆ ⁺ (89), 328.09006 (20)	Licoricone
U17	C ₂₁ H ₂₄ O ₆ (0.362)	371.15009	109.02789 – C ₆ H ₅ O ₂ ⁻ (100), 231.06561 – C ₁₃ H ₁₁ O ₄ ⁻ (22)	373.16470	149.05991 – C ₉ H ₉ O ₂ ⁺ (48), 151.07552 – C ₉ H ₁₁ O ₂ ⁺ (18), 179.07042 – C ₁₀ H ₁₁ O ₃ ⁺ (100), 180.07372 (10), 207.06541 – C ₁₁ H ₁₁ O ₄ ⁺ (19)	n.i. B-ring 3,3-DMA prenylated
U21	C ₂₂ H ₂₂ O ₆ (0.274)	381.13458	148.01512 – C ₈ H ₄ O ₃ ⁻ (16), 149.02321 – C ₈ H ₅ O ₃ ⁻ (13), 201.01846 – C ₁₁ H ₅ O ₄ ⁻ (25), 279.03003 – C ₁₆ H ₇ O ₅ ⁻ (19), 352.09024 (22)	383.14902	69.07080 – C ₅ H ₉ ⁺ (19), 123.04446 – C ₇ H ₇ O ₂ ⁺ (18), 149.02367 – C ₈ H ₅ O ₃ ⁺ (13), 243.10194 – C ₁₅ H ₁₅ O ₃ ⁺ (14), 283.06058 – C ₁₆ H ₁₁ O ₅ ⁺ (13), 284.06833 – C ₁₆ H ₁₂ O ₅ ⁺ (73), 285.07187 (15), 286.08392 – C ₁₆ H ₁₄ O ₅ ⁺ (19),	Glycyrrin

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (m/z)	MS ² NI mode m/z (R.A.)	[M+H] ⁺ (m/z)	MS ² PI mode m/z (R.A.)	Tentatively identified compound
U22	C ₂₆ H ₃₂ O ₅ (-1.107)	423.21741	307.09692 – C ₁₉ H ₁₅ O ₄ ⁻ (19), 323.09213 – C ₁₉ H ₁₅ O ₅ ⁻ (13), 337.10782 – C ₂₀ H ₁₇ O ₅ ⁻ (19), 351.08716 – C ₂₀ H ₁₅ O ₆ ⁻ (100), 124.01505 – C ₆ H ₄ O ₃ ⁻ (14), 125.09564 (10), 149.09575 – C ₁₀ H ₁₃ O ⁻ (16), 151.07504 – C ₉ H ₁₁ O ₂ ⁻ (13), 177.09103 – C ₁₁ H ₁₃ O ₂ ⁻ (10), 193.08595 – C ₁₁ H ₁₃ O ₃ ⁻ (100), 194.08934 (10), 203.10681 – C ₁₃ H ₁₅ O ₂ ⁻ (34), 207.10175 – C ₁₂ H ₁₅ O ₃ ⁻ (11), 229.08632 – C ₁₄ H ₁₃ O ₃ ⁻ (46)	425.23178	257.08102 – C ₁₅ H ₁₃ O ₄ ⁺ (17), 269.04483 – C ₁₅ H ₉ O ₅ ⁺ (10), 269.08109 – C ₁₆ H ₁₃ O ₄ ⁺ (11), 271.06058 – C ₁₅ H ₁₁ O ₅ ⁺ (13), 69.07077 – C ₃ H ₉ ⁺ (15), 123.04447 – C ₇ H ₇ O ₂ ⁺ (11), 135.04433 – C ₈ H ₇ O ₂ ⁺ (100), 137.06001 – C ₈ H ₉ O ₂ ⁺ (32), 139.03922 – C ₇ H ₇ O ₃ ⁺ (13), 147.04428 – C ₉ H ₇ O ₂ ⁺ (24), 149.06003 – C ₉ H ₉ O ₂ ⁺ (10), 153.05490 – C ₈ H ₉ O ₃ ⁺ (23), 159.04449 – C ₁₀ H ₇ O ₂ ⁺ (10), 161.05997 – C ₁₀ H ₉ O ₂ ⁺ (22), 299.09189 – C ₁₇ H ₁₅ O ₅ ⁺ (100), 300.09512 (23) 313.14383 – C ₁₉ H ₂₁ O ₄ ⁺ (16), 383.14957 – C ₂₂ H ₂₃ O ₆ ⁺ (10), 165.05489 – C ₉ H ₉ O ₃ ⁺ (83), 167.07056 – C ₉ H ₁₁ O ₃ ⁺ (18), 179.07054 – C ₁₀ H ₁₁ O ₃ ⁺ (50), 189.09123 – C ₁₂ H ₁₃ O ₂ ⁺ (13), 191.07050 – C ₁₁ H ₁₁ O ₃ ⁺ (11), 191.10696 – C ₁₂ H ₁₅ O ₂ ⁺ (44), 221.11755 – C ₁₃ H ₁₇ O ₃ ⁺ (31), 253.08617 – C ₁₆ H ₁₃ O ₃ ⁺ (14), 313.10727 – C ₁₈ H ₁₇ O ₅ ⁺ (18)	Licoricidin
U23	C ₂₂ H ₂₄ O ₅ (0.135)	383.15027 ^(d)	109.02785 – C ₆ H ₅ O ₂ ⁻ (17), 121.02793 – C ₇ H ₅ O ₂ ⁻ (19), 148.01518 – C ₈ H ₄ O ₃ ⁻ (50), 149.05931 – C ₉ H ₉ O ₂ ⁻ (14), 161.02321 – C ₉ H ₅ O ₃ ⁻ (10), 175.03867 – C ₁₀ H ₇ O ₃ ⁻ (12), 203.07031 – C ₁₂ H ₁₁ O ₃ ⁻ (74), 204.07393 (10), 205.08633 – C ₁₂ H ₁₃ O ₃ ⁻ (14), 133.06445 – C ₉ H ₉ O ⁻ (15), 146.93719 (13), 151.07506 – C ₉ H ₁₁ O ₂ ⁻ (39), 183.91219 (35), 201.09138 – C ₁₃ H ₁₃ O ₂ ⁻ (16), 241.90318 (11), 243.10234 – C ₁₅ H ₁₅ O ₃ ⁻ (21), 267.10208 – C ₁₇ H ₁₅ O ₃ ⁻ (17), 269.08197 – C ₁₆ H ₁₃ O ₄ ⁻ (12), 284.10556 – C ₁₇ H ₁₆ O ₄ ⁻ (14), 217.04987 – C ₁₂ H ₉ O ₄ ⁻ (10), 256.03741 – C ₁₄ H ₈ O ₅ ⁻ (40), 281.11819 – C ₁₈ H ₁₇ O ₃ ⁻ (13), 282.05295 – C ₁₆ H ₁₀ O ₅ ⁻ (12), 297.07623 – C ₁₇ H ₁₃ O ₅ ⁻ (22), 309.11240 – C ₁₉ H ₁₇ O ₄ ⁻ (10), 325.10797 – C ₁₉ H ₁₇ O ₅ ⁻ (100), 326.11118 (24), 340.13162 – C ₂₀ H ₂₀ O ₅ ⁻ (13)	367.15405	147.04428 – C ₉ H ₇ O ₂ ⁺ (17), 165.05490 – C ₈ H ₉ O ₃ ⁺ (21), 297.07614 – C ₁₇ H ₁₃ O ₅ ⁺ (40), 309.07605 – C ₁₈ H ₁₃ O ₅ ⁺ (100), 310.08938 (23), 337.10739 – C ₂₀ H ₁₇ O ₅ ⁺ (15), 367.15454 – C ₂₂ H ₂₃ O ₅ ⁺ (28)	Dehydroglyasperin D
U25	C ₂₅ H ₂₆ O ₆ (0.555)	421.16611	133.06445 – C ₉ H ₉ O ⁻ (15), 146.93719 (13), 151.07506 – C ₉ H ₁₁ O ₂ ⁻ (39), 183.91219 (35), 201.09138 – C ₁₃ H ₁₃ O ₂ ⁻ (16), 241.90318 (11), 243.10234 – C ₁₅ H ₁₅ O ₃ ⁻ (21), 267.10208 – C ₁₇ H ₁₅ O ₃ ⁻ (17), 269.08197 – C ₁₆ H ₁₃ O ₄ ⁻ (12), 284.10556 – C ₁₇ H ₁₆ O ₄ ⁻ (14), 297.04004 – C ₁₆ H ₉ O ₆ ⁻ (14), 309.04004 – C ₁₇ H ₉ O ₆ ⁻ (35), 311.05588 – C ₁₇ H ₁₁ O ₆ ⁻ (14), 323.05560 – C ₁₈ H ₁₁ O ₆ ⁻ (49), 352.09528 – C ₂₀ H ₁₆ O ₆ ⁻ (47), 353.09833 (15), 353.17526 – C ₂₂ H ₂₅ O ₄ ⁻ (18), 365.10220 – C ₂₁ H ₁₇ O ₆ ⁻ (12), 421.16547 – C ₂₅ H ₂₅ O ₆ ⁻ (100), 422.16891 (37)	423.18045	311.05515 – C ₁₇ H ₁₁ O ₆ ⁺ (100), 312.05850 (20)	Glyasperin A
U26	C ₂₆ H ₃₀ O ₅ (0.022)	421.20248	n.d.	423.21661	135.04430 – C ₈ H ₇ O ₂ ⁺ (17), 137.05995 – C ₈ H ₉ O ₂ ⁺ (12), 149.05994 – C ₉ H ₉ O ₂ ⁺ (39), 165.05484 – C ₉ H ₉ O ₃ ⁺ (20), 173.09637 – C ₁₂ H ₁₃ O ⁺ (18), 191.10686 – C ₁₂ H ₁₅ O ₂ ⁺ (100), 192.11024 (14)	1-Methoxyficifolinol
U27	C ₂₁ H ₂₀ O ₅ (0.056)	n.d.	n.d.	353.13837	267.06531 – C ₁₆ H ₁₁ O ₄ ⁺ (100), 268.06873 (18), 297.07593 – C ₁₇ H ₁₃ O ₅ ⁺ (76), 298.07922 (16)	Gancaonin A
U28	C ₂₂ H ₂₄ O ₆ (0.117)	383.15036	n.d.	385.16461	137.05991 – C ₈ H ₉ O ₂ ⁺ (100), 205.04982 – C ₁₁ H ₉ O ₄ ⁺ (19), 311.09161 – C ₁₈ H ₁₅ O ₅ ⁺ (21)	n.i. C6 3,3-DMA prenylated without <i>ortho</i> -OCH ₃
U29	n.d.	775.34955	n.d.	777.36298	n.d.	n.i. double 3,3-DMA prenylated

No.	Molecular formula (error Δ ppm)	[M-H] ⁺ (<i>m/z</i>)	MS ² NI mode <i>m/z</i> (R.A.)	[M+H] ⁺ (<i>m/z</i>)	MS ² PI mode <i>m/z</i> (R.A.)	Tentatively identified compound
U31	C ₂₇ H ₃₄ O ₅ (0.340)	437.23337	177.09093 – C ₁₁ H ₁₃ O ₂ ⁻ (26), 203.10678 – C ₁₃ H ₁₅ O ₂ ⁻ (100), 204.11020 (15), 215.10695 – C ₁₄ H ₁₅ O ₂ ⁻ (14), 219.10182 – C ₁₃ H ₁₅ O ₃ ⁻ (20),	439.24805	69.07082 – C ₅ H ₉ ⁺ (43), 135.04442 – C ₈ H ₇ O ₂ ⁺ (50), 137.06006 – C ₈ H ₉ O ₂ ⁺ (10), 161.05997 – C ₁₀ H ₉ O ₂ ⁺ (19), 167.07062 – C ₉ H ₁₁ O ₃ ⁺ (100),	179.07063 – C ₁₀ H ₁₁ O ₃ ⁺ (29), 181.08629 – C ₁₀ H ₁₃ O ₃ ⁺ (26), 191.10706 – C ₁₂ H ₁₅ O ₂ ⁺ (30), 193.08638 – C ₁₁ H ₁₃ O ₃ ⁺ (16), 235.13330 – C ₁₄ H ₁₉ O ₃ ⁺ (17)

n.d. Not detected

G. Determination of growth delay

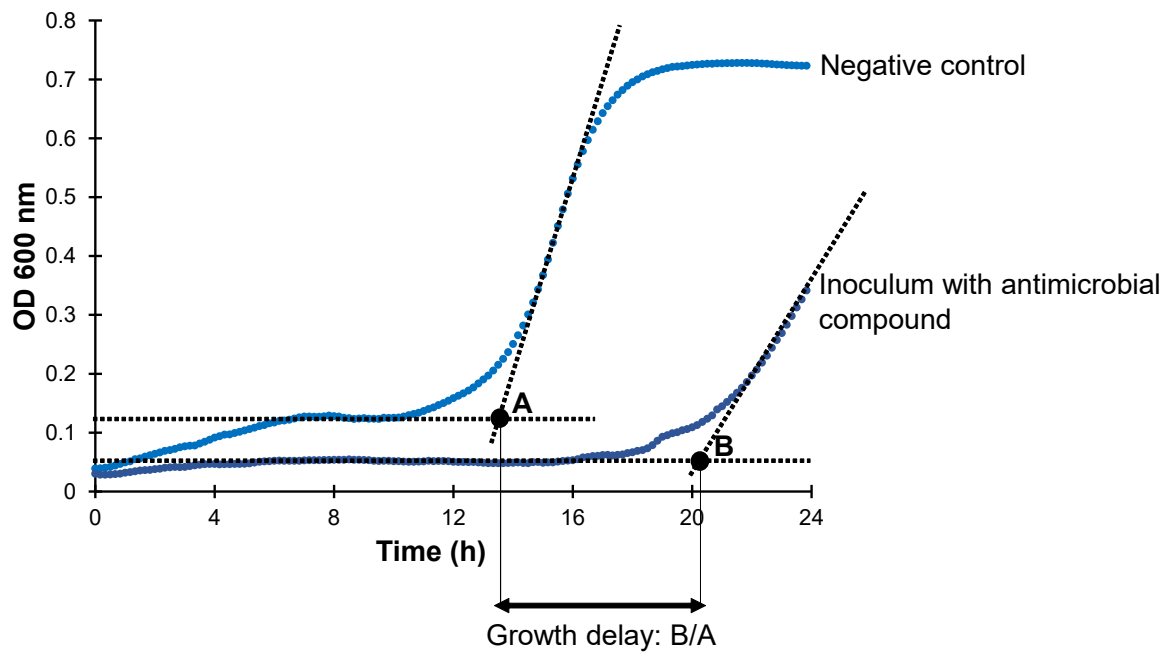


Figure G1. Determination of growth delay. Growth delay was defined as the ratio between intercept B (inoculum in the presence of antimicrobial compound) and intercept A (inoculum in the absence of antimicrobial compound or negative control).

H. Quantification of prenylated phenolics in EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent

Table H1. Quantification of (prenylated) phenolics in EtOAc extract of *G. glabra*, *G. inflata*, and *G. uralensis* spent.

No ^(a)	Compound	<i>G. glabra</i> Concentration $\pm$ SD (mg g ⁻¹ dry extract)	<i>G. inflata</i> Concentration $\pm$ SD (mg g ⁻¹ dry extract)	<i>G. uralensis</i> Concentration $\pm$ SD (mg g ⁻¹ dry extract)
G-I-U 1	Liquiritigenin	3.38 $\pm$ 0.26	7.19 $\pm$ 0.19	28.55 $\pm$ 1.09
G-I-U-2	Isoliquiritigenin	2.06 $\pm$ 0.14	5.03 $\pm$ 0.16	9.08 $\pm$ 0.41
G-I-U-3	Formononetin	2.06 $\pm$ 0.16	1.74 $\pm$ 0.11	1.54 $\pm$ 0.06
G4	7,4'-Dihydroxy-8-prenylflavone	0.83 $\pm$ 0.33		
G-I-5	Glabrene	5.06 $\pm$ 0.26	2.62 $\pm$ 0.09	
G6	Phaseollinisoflavan	1.21 $\pm$ 0.09		
G7	n.i. Not prenylated	3.41 $\pm$ 0.15		
G8	Glabrone	(b)		
G-I-9	Glabrocoumarin	1.04 $\pm$ 0.20	10.16 $\pm$ 0.45	
G10	Licoagrochalcone C	2.39 $\pm$ 0.25		
G-I-11	Glabridin	8.68 $\pm$ 0.71	3.59 $\pm$ 0.25	
G12	3-Hydroxyglabrol	1.24 $\pm$ 0.09		
G13	Phaseollin	2.56 $\pm$ 0.23		
G14	n.i. B-ring 3,3-DMA prenylated	(b)		
G15	n.i. 2,2-DMP prenylated	1.46 $\pm$ 0.09		
G16	Scanderone	1.39 $\pm$ 0.13		
G17	Kanzonol E	(b)		
G18	Kanzonol Y or Glycybridin C	5.93 $\pm$ 0.56		
G19	n.i. At least single 3,3-DMA prenylated	(b)		
G20	n.i. Not prenylated	1.03 $\pm$ 0.20		
G-I-21	Licoflavone B	0.63 $\pm$ 0.16	1.88 $\pm$ 0.16	
G22	3'-Hydroxy-4'-methoxyglabridin	2.68 $\pm$ 0.32		
G-I-23	Glabrol	4.47 $\pm$ 0.47	20.86 $\pm$ 1.13	
G24	Kanzonol Y or Glycybridin C	4.78 $\pm$ 1.32		
G25	Licocoumarin A	3.77 $\pm$ 0.15		
G-I-26	Gancaonin E	2.84 $\pm$ 0.26	8.82 $\pm$ 0.30	
G27	Kanzonol X	(b)		
G28	4'-Methoxyglabridin	2.33 $\pm$ 0.20		
G29	Kanzonol E isomer	4.12 $\pm$ 0.18		
G30	n.i. Double 3,3-DMA prenylated	1.76 $\pm$ 0.16		
G31	8-Prenylphaseollinisoflavan	3.00 $\pm$ 0.34		
G32	n.i. Double 3,3-DMA prenylated	4.72 $\pm$ 3.39		
G33	Hispaglabridin A	6.51 $\pm$ 0.63		
G34	n.i. Double 3,3-DMA prenylated			
G35	Glyinflanin A	2.26 $\pm$ 0.21		
G36	n.i. B-ring single 3,3-DMA prenylated	5.74 $\pm$ 0.35		
G37	3-Oxoglycyrrhithenic acid	(b)		
G38	n.i. At least single 2,2-DMP prenylated	2.81 $\pm$ 0.23		
G39	Hispaglabridin B	5.10 $\pm$ 0.49		
G40	n.i. Not prenylated	1.35 $\pm$ 0.18		
G41	n.i. Double chain prenylated	2.13 $\pm$ 0.34		
I-U-4	Naringenin		1.31 $\pm$ 0.07	2.58 $\pm$ 0.11
I-U-6	Echinatin		(b)	(b)
I7	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B		2.03 $\pm$ 0.10	
I-U-8	Licoisoflavanone		1.17 $\pm$ 0.27	1.72 $\pm$ 0.20
I10	n.i. A-ring 3,3-DMA prenylated without <i>ortho</i> -OCH ₃		2.78 $\pm$ 0.08	
I-U-12	Licoisoflavone B or Sophoraisoflavone A or		2.40 $\pm$ 0.10	5.06 $\pm$ 0.36

	Semilicoisoflavone B		
I13	Licoflavone C	2.03 ± 0.08	
I-U-14	Glyasperin C	1.91 ± 0.12	2.64 ± 0.57
I-U-15	Uralenin	6.79 ± 0.17	1.39 ± 0.03
I-U-16	Licoisoflavone A	4.80 ± 0.45	1.71 ± 0.21
I17	Licochalcone A	23.7 ± 1.01	
I-U-18	3'-Prenylgenistein (Isowighteone)	1.71 ± 0.11	4.07 ± 0.08
I-U-19	Glycyrol	(b)	(b)
I-U-20	Licoisoflavone B or Sophoraisoflavone A or Semilicoisoflavone B	23.69 ± 1.71	2.67 ± 0.28
I22	Isoderrone	1.70 ± 0.06	
I-U-24	Glyasperin D	2.12 ± 0.04	3.09 ± 0.18
I25	Macarangaflavanone B (Paratocarpin L)	7.95 ± 1.28	
I27	n.i. Double 3,3-DMA and 2,2-DMP prenylated	4.28 ± 0.26	
I28	n.i. Double 3,3-DMA prenylated	3.38 ± 0.12	
I29	Gancaonin E isomer	2.74 ± 0.09	
I-U-30	2'-Hydroxy- Isolupalbingenin ((Iso)angustone A)	9.82 ± 0.32	6.72 ± 0.53
I31	n.i. Double 3,3-DMA prenylated	(b)	
I32	Euchrenone A5	1.75 ± 0.16	
I33	Glyurallin B	3.90 ± 0.11	
I-U-34	6,8-Diprenylgenistein	4.57 ± 0.22	4.24 ± 0.16
I35	2'-Hydroxy- Isolupalbingenin ((Iso)angustone A)	(b)	
I36	Angustone B	8.31 ± 0.44	
U5	Glyasperin B		1.42 ± 0.11
U7	n.i. O-3,3-DMA prenylated		14.20 ± 0.60
U9	Glycycoumarin		18.52 ± 1.25
U10	Glycyrrhisoflavone		4.89 ± 0.25
U11	n.i. C6 3,3-DMA prenylated without <i>ortho</i> -OCH3		7.65 ± 0.63
U13	Licoricone		(b)
U17	n.i. B-ring 3,3-DMA prenylated		5.05 ± 0.32
U21	Glycyrin		3.67 ± 0.36
U22	Licoricidin		32.64 ± 2.07
U23	Dehydroglyasperin D		4.62 ± 0.60
U25	Glyasperin A		5.90 ± 0.23
U26	1-Methoxyficifolinol		4.72 ± 0.50
U27	Gancaonin A		1.43 ± 0.14
U28	n.i. C6 3,3-DMA prenylated without <i>ortho</i> -OCH3		2.67 ± 1.63
U29	n.i. double 3,3-DMA prenylated		3.83 ± 0.39
U31	Licorisoflavan A		10.04 ± 0.61
	Total	104.7 ± 12.5	186.7 ± 9.8 196.3 ± 12.1

^(a)Numbering correspond to annotation in **Table S3**.

^(b)Quantification based only on the previous compound due to co-elution of UV peaks.

I. Minimum inhibitory prenylated phenolics concentrations and minimum bactericidal/fungicidal prenylated phenolics concentrations

Table I1. Minimum inhibitory prenylated phenolics concentrations (MIPPCs) and minimum bactericidal/fungicidal prenylated phenolics concentrations (MBPPC/MFPPC) of liquorice spent extracts.

Bacteria/ Yeasts	<i>G. glabra</i>		<i>G. inflata</i>		<i>G. uralensis</i>	
	MIPPC (LR ^a ±SD ^b)	MBPPC/MFPPC (LR±SD)	MIPPC (LR±SD)	MBPPC/MFPPC (LR±SD)	MIPPC (LR±SD)	MBPPC/MFPPC (LR±SD)
BACTERIA						
<i>L. buchneri</i>						
ATCC 4005	24-48 (2.22±1.54)	24-96 (3.14±0.79)	42.8 (3.55±0.98)	42.8 (3.55±0.98)	7.8 (2.66±2.54)	7.8-15.6 (4.65±0.78)
L4	24-48 (1.59±1.33)	24-96 (3.56±1.34)	42.8 (4.48±1.12)	42.8 (4.48±1.12)	7.8-15.6 (3.94±0.39)	7.8-15.6 (3.94±0.39)
<i>S. mutans</i>						
ATCC 27175	>96 (n.d. ^c)	>192 (n.d.)	17.1 (0.59±0.35)	>171 (n.d.)	38.8 (0.75±0.06)	155 (2.58±0.12)
<i>S. aureus</i>						
ATCC 25923	7.2 (3.71±0.01)	7.2 (3.71±0.01)	4.3-8.6 (1.86±2.80)	8.6-17.1 (4.88±0.34)	3.9 (1.92±1.75)	3.9-7.8 (3.61±1.43)
<i>E. coli</i>						
K12	>192 (n.d.)	>192 (n.d.)	>342 (n.d.)	>342 (n.d.)	>310 (n.d.)	>310 (n.d.)
O54:H21	>192 (n.d.)	>192 (n.d.)	>342 (n.d.)	>342 (n.d.)	>310 (n.d.)	>310 (n.d.)
O88:H8	>192 (n.d.)	>192 (n.d.)	>342 (n.d.)	>342 (n.d.)	>310 (n.d.)	>310 (n.d.)
YEASTS						
<i>Y. lipolytica</i>						
Food isolate	>192 (n.d.)	>192 (n.d.)	>342 (n.d.)	>342 (n.d.)	>310 (n.d.)	>310 (n.d.)
<i>Z. parabailli</i>						
ATCC 60483	>192 (n.d.)	>192 (n.d.)	>342 (n.d.)	>342 (n.d.)	>310 (n.d.)	>310 (n.d.)
UL 3699	>192 (n.d.)	>192 (n.d.)	>342 (n.d.)	>342 (n.d.)	>310 (n.d.)	>310 (n.d.)

^aLR = log reduction of the initial inoculum after 24h incubation; ^bSD = standard deviation; ^cn.d. = not determined.

J. Descriptor values of prenylated phenolics associated with antifungal activity

Table J1. Descriptor values of prenylated (iso)flavonoids associated with antifungal activity against *Z. parabailli* and *Y. lipolytica*; hydrophobic integrity moment (V_{surf_ID7})^a, the octanol/water distribution coefficient at pH 6.5 ($LogD$), and the molecular flexibility index ($Kierflex$). All descriptors, except $LogD$, were calculated with MOE. For all compounds a conformational search (LowModeMD, RSM gradient 0.1 kcal/mol/Å) and energy minimization was performed using MOPAC force field (RSM gradient 0.01 kcal/mol/Å). $LogD$ was calculated with MarvinSketch 20.3. MIC values were adapted from Kalli *et al.*¹³ MICs of glycycomarin and licochalcone A were confirmed in this research.

Compound	MIC ($\mu\text{g mL}^{-1}$)	V_{surf_ID7} (Å)	$LogD$ (pH 6.5)	$Kierflex$
6-Prenylgenistein (wighteone)	3.13-6.25	1.1	4.5	3.5
3'-Prenylgenistein (isowighteone)	6.25-12.5	0.5	4.5	3.5
Glabridin	6.25-12.5	1.1	4.1	2.9
Luteone	12.5	0.8	4.0	3.7
Dehydroglyceollin I	12.5-25	0.9	3.9	2.2
Glabrene	25	0.9	4.0	2.7
4'-OH-Methylglabridin	25	0.9	4.2	3.3
Neobavaisoflavone	50	0.4	4.0	3.3
3'-OH-4'-OH-methylglabridin	>>25	1.3	3.9	3.5
8-Prenylgenistein (lupiwighteone)	>>25	1.0	4.4	3.5
Dehydroglyceollin III	>>25	0.6	3.9	2.3
Glabrol	>>25	0.5	5.9	5.0
Hispaglabridin B	>>25	0.5	5.3	3.4
6,8-Diprenylgenistein	>>25	1.3	6.0	5.0
6'-Prenylpiscidone	>>25	1.5	5.7	5.9
Glycycomarin	100	1.1	4.0	4.1
Licochalcone A	>100	0.5	4.8	4.2

^aThe hydrophobic integrity moment is a measure of unbalance between the centre of mass of a molecule and the barycentre of the hydrophobic regions; *e.g.* a small integrity moment indicates that hydrophobic moieties are either close to the centre of mass or they balance at opposite ends of the molecule, so that the resulting barycentre is close to the centre of the molecule.¹⁴

K. Growth delay of liquorice extracts and time to detection of species specific marker compounds against various microorganisms

Table K1. Growth delay and time to detection (TTD) for EtOAc extracts of *G. glabra*, *G. inflata*, and *G. uralensis* spent, and species-specific marker compounds glabridin (Glab), licochalcone A (LicoA), and glycycomarin (Glycy). Growth delay is expressed as ratio between start of microbial growth in the experiment with microbial growth of bacterial/yeast inoculum (**Figure G1**).

Bacteria/Yeasts	Concentration (µg mL ⁻¹)	GD (microbial growth/microbial growth inoculum)			TTD (h)			
		<i>G. glabra</i>	<i>G. inflata</i>	<i>G. uralensis</i>	Concentration (µg mL ⁻¹)	Glab	LicoA	Glycy
BACTERIA								
<i>L. buchneri</i>								
ATCC 4005					<i>Negative control: 22.3±7.8</i>			
	25	1.2	1.4	1.4	3.125	18.8	15.5	14.0
	50	1.3	1.9	>4.4±1.5	6.25	16.8	42.3±26.8	15.3
	100	1.7	3.5±1.8	>4.4±1.5	12.5	49.8±19.6	>72	29.8±21.0
	250	4.0±1.5	>4.4±1.5	>4.4±1.5	25	>72	45.7±37.2	>72
	500	>4.4±1.5	>4.4±1.5	>5.6	50	>72	>72	>72
	1000	>4.4±1.5	>5.6	>5.6	100	>72	>72	>72
	2000	3.8±1.6	n.t. ^b	n.t.				
L4					<i>Negative control: 23.1±0.3</i>			
	25	1.0	1.1	1.3	3.125	22.5	56.7±26.5	22.7
	50	4.1	1.3	>3.3±0.2	6.25	47.8±34.3	>72	37.9±29.7
	100	1.3	2.5±0.4	>3.3±0.2	12.5	61.9±17.4	>72	>72
	250	>3.3±0.2	>3.3±0.2	>3.3±0.2	25	>72	>72	58.4±23.5
	500	>3.3±0.2	>3.3±0.2	>3.0	50	>72	>72	>72
	1000	>3.3±0.2	>3.0	>3.0	100	>72	>72	>72
	2000	>3.4±0.2	n.t.	n.t.				
<i>S. mutans</i>								
ATCC 27175					<i>Negative control: 10.5±1.0</i>			
	50	1.1±0.0	>2.2±0.2	1.9±0.4	3.125	10.7±0.6	11.8±1.1	10.6±0.8
	100	1.3±0.1	>2.2±0.2	>2.2±0.2	6.25	12.3±0.7	18.2±5.0	11.6±1.0
	250	1.8±0.1	>2.2±0.2	>2.2±0.2	12.5	>24	>24	17.3±5.8
	500	>2.2±0.2	>2.2±0.2	>2.2±0.2	25	>24	>24	>24
	1000	>2.2±0.2	>2.2±0.2	>2.2±0.2	50	>24	>24	>24
	2000	>2.2±0.2	>2.2±0.2	>2.2±0.2	100	>24	>24	>24
<i>S. aureus</i>								
ATCC 25923					<i>Negative control: 14.4±2.7</i>			
	3.125	n.t.	n.t.	16.6±1.8 ^a	3.125	12.3	15.3	17.7
	6.25	n.t.	n.t.	17.4±2.0 ^a	6.25	15.9±4.0	>24	>24

	12.5	n.t.	21.8±1.9 ^a	>24 ^a	12.5	>24	>24	>24
	16.7	n.t.	n.t.	22.0±2.83 ^a	25	>24	>24	>24
	20.8	n.t.	n.t.	>24 ^a	50	>24	>24	>24
	25	21.8±3.1 ^a	>24 ^a	>24 ^a				
	50	>24 ^a	>24 ^a	>24 ^a				
	75	>24 ^a	>24 ^a	n.t.				
	100	>24 ^a	>24 ^a	>24 ^a				
	125	>24 ^a	n.t.	n.t.				
	150	>24 ^a	n.t.	n.t.				
	175	>24 ^a	n.t.	n.t.				
	200	>24 ^a	>24 ^a	>24 ^a				
	400	>24 ^a	>24 ^a	>24 ^a				
YEASTS								
<i>Y. lipolytica</i>								
Food isolate					<i>Negative control: 14.3±0.5</i>			
	50	1.2	1.4	1.5	3.125	14.5	14.3	14.7
	100	0.8	1.6	1.1	6.25	12.3±1.1	14.5	12.7
	250	0.9	1.3	1.5	12.5	16.3±2.1	16.2	13.2
	500	1.3±0.1	1.3±0.1	1.3±0.2	25	40.6±10.5	18.1±0.8	16.3±0.4
	1000	1.7±0.0	1.5±0.5	2.1±0.4	50	>48	20.7±1.9	28.0±6.4
	2000	2.8±1.6	2.7±0.7	3.0±1.3	100	>48	24.3±1.1	>48
<i>Z. parabailli</i>								
ATCC 60483					<i>Negative control: 10.7±1.3</i>			
	50	1.1	1.1	1.2	3.125	9.5	10.2	9.7
	100	1.1	1.2	1.1	6.25	13.7±3.1	11.5	10.2
	250	1.2	1.3	1.1	12.5	27.2±6.0	15.7	10.8
	500	1.3	1.4	1.4	25	>48	17.8	11.5
	1000	1.3	1.6	1.6	50	>48	20.5±1.2	16.0±3.3
	2000	1.3±0.1	1.7±0.1	2.0±0.1	100	>48	n.t.	35.1±13.4
UL 3699					<i>Negative control: 13.3±0.9</i>			
	50	1.1	1.1	1.0	3.125	13.2	14.3	13.2
	100	1.1	1.3	1.1	6.25	18.7±2.0	17.2	12.8
	250	1.1	1.6	1.5	12.5	45.3±4.7	33.2	12.8
	500	1.1	1.9	2.0	25	>48	42.2±5.2	13.7
	1000	1.2	2.2	2.5	50	>48	46.5±2.6	19.5±2.0
	2000	1.1±0.1	2.3±0.2	2.8±0.1	100	>48	>48	>48

^a Time to detection (TTD) instead of growth delay; ^b Not tested.

L. Blank measurements of liquorice spent extracts and species specific marker compounds

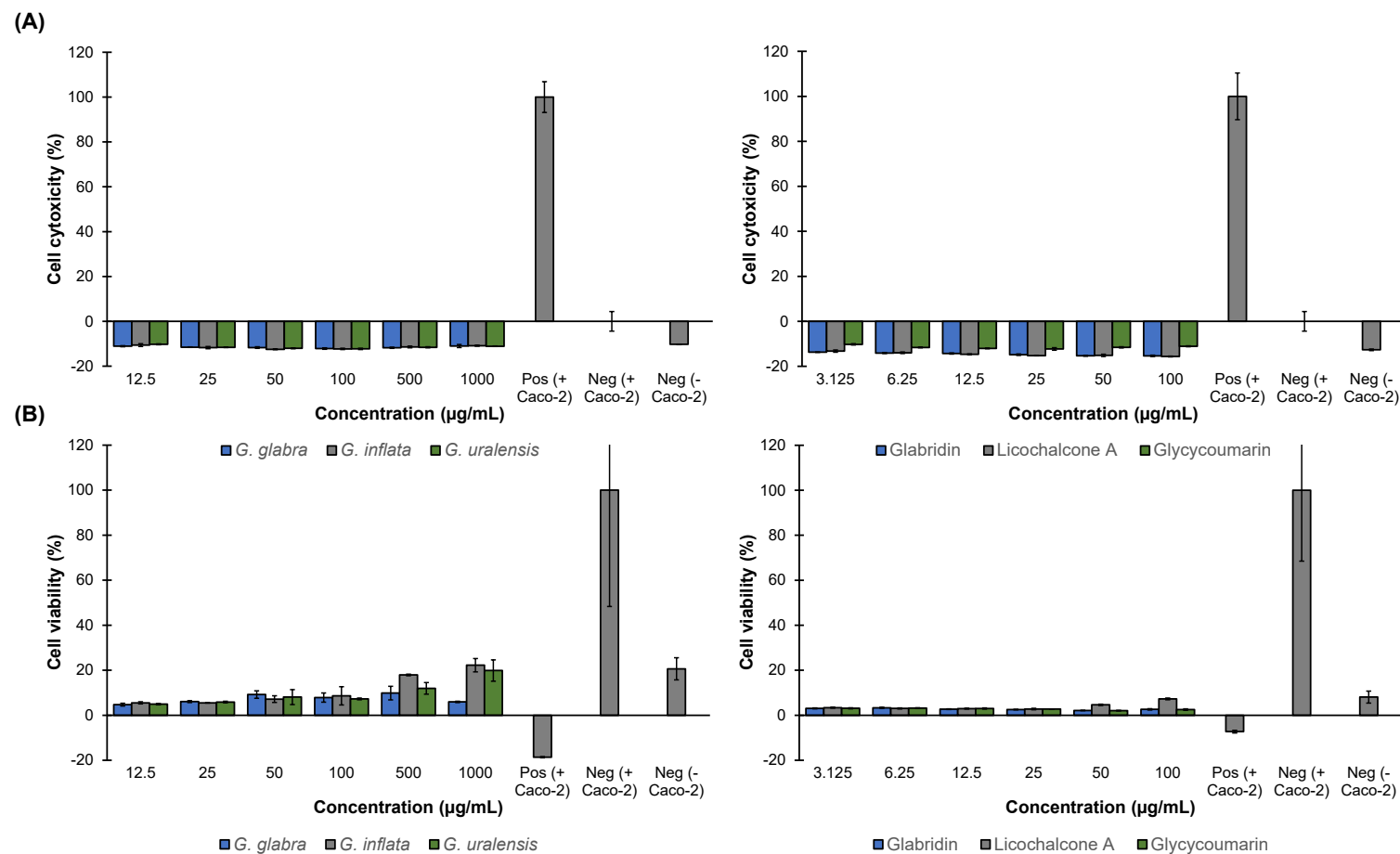


Figure L1. Blank measurements of cell cytotoxicity (A) and cell viability (B) of EtOAc extracts of *Glycyrrhiza glabra*, *G. inflata*, and *G. uralensis* spent, and species specific marker compounds glabridin, licochalcone A, and glycycomarin without Caco-2 cells. No significant differences were observed compared to the negative control without Caco-2 cells (Neg [- Caco-2]).

M. Control experiments microorganism growth in the presence of DMSO

Table M1. Microbial count after 24/72 h incubation time (Table D1) without and in the presence of DMSO.

Microorganism	Microbial count $\pm$ SD (log CFU mL ⁻¹) - DMSO	Microbial count $\pm$ SD (log CFU mL ⁻¹) + max. 2 % (v/v) DMSO
<i>Lactobacillus buchneri</i>		
ATCC 4005	7.8 $\pm$ 0.9	7.6 $\pm$ 0.7
UL	8.7 $\pm$ 0.3	8.7 $\pm$ 0.2
<i>Streptococcus mutans</i>		
ATCC 27175	9.0 $\pm$ 0.1	9.0 ^(a)
<i>Staphylococcus aureus</i>		
ATCC 25923	8.3 $\pm$ 0.6	8.1 $\pm$ 0.3
<i>Escherichia coli</i>		
K12	9.5 ^(a)	10.1 ^(a)
O54:H21	9.8 $\pm$ 0.4	9.6 $\pm$ 0.3
O88:H8	9.7 $\pm$ 0.4	9.9 $\pm$ 0.4
<i>Yarrowia lipolytica</i>		
Food isolate	7.2 $\pm$ 0.7	6.8 $\pm$ 0.1
<i>Zygosaccharomyces parabailli</i>		
ATCC 60483	8.0 $\pm$ 0.1	8.1 $\pm$ 0.1
UL 3699	7.8 $\pm$ 0.2	7.9 $\pm$ 0.2

^(a)Measured in one biological replicate.

N. DMSO cytotoxicity in Caco-2 cells

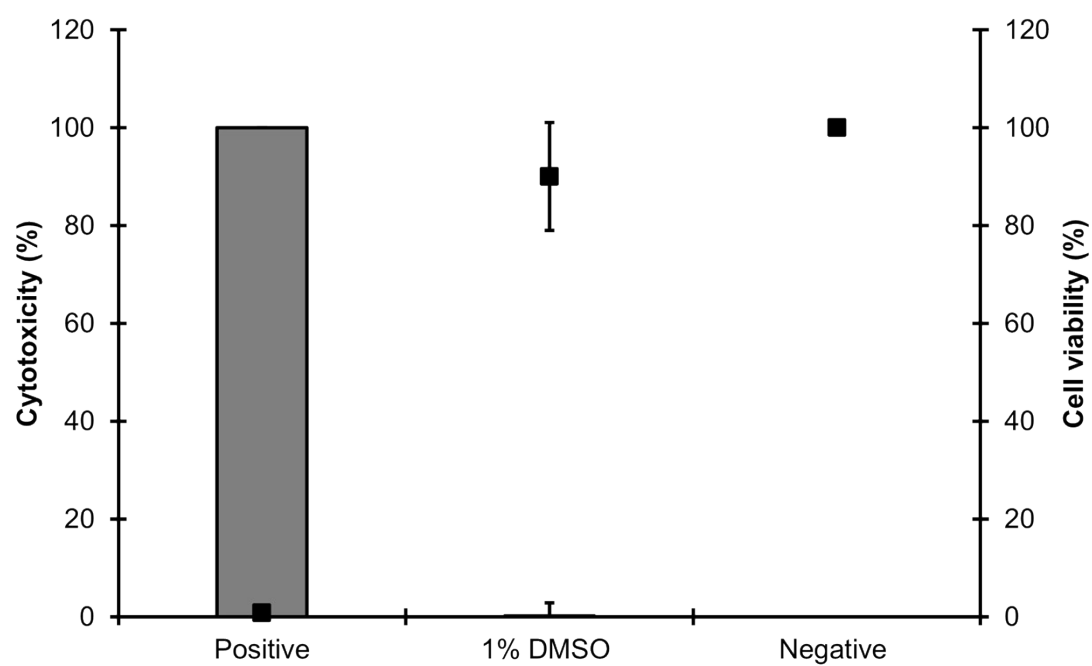


Figure N1. Cell cytotoxicity (bars, primary vertical axis) and cell viability (squares, secondary vertical axis) after 4 h incubation with 1 % (v/v) DMSO in Caco-2 cells. Values are means $\pm$ standard deviation, measured in three biological replicates.

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